



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:18 PM UTC

PDB ID : 2XKA / pdb_00002xka
Title : Crystal structure of a GTPyS-form protofilament of *Bacillus thuringiensis* serovar israelensis TubZ
Authors : Aylett, C.H.S.; Lowe, J.
Deposited on : 2010-07-07
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

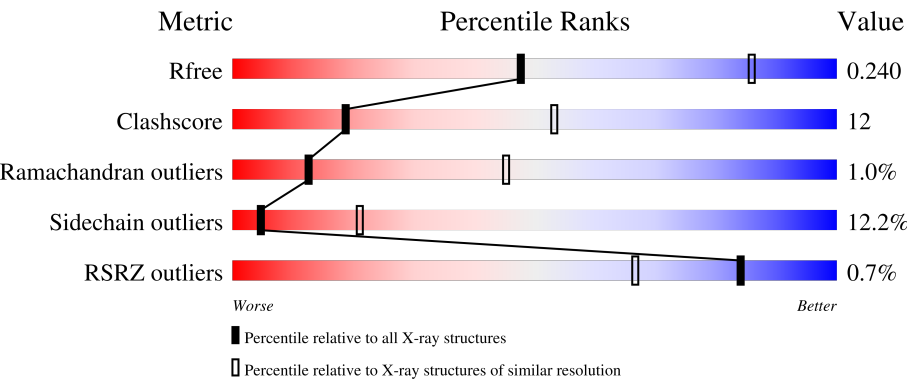
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	421	% 69% 23% • 5%
1	B	421	67% 24% • 5%
1	C	421	% 68% 25% • •
1	D	421	67% 25% • 5%
1	E	421	% 67% 23% • 6%

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Mol	Chain	Length	Quality of chain
1	F	421	% 69% 25% 5%
1	G	421	69% 25% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22638 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

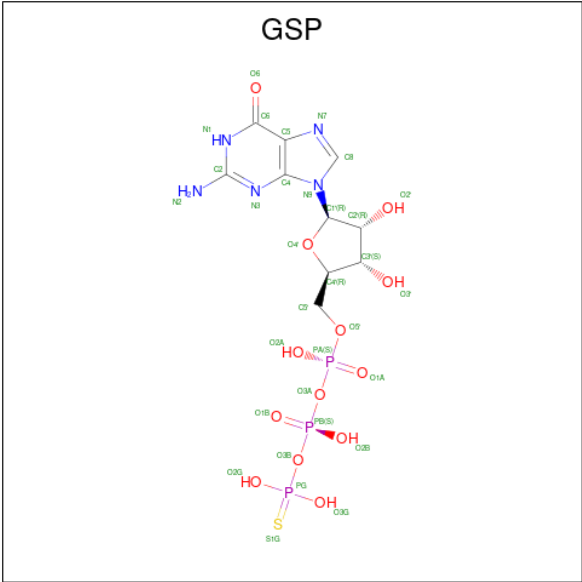
- Molecule 1 is a protein called FTSZ/TUBULIN-RELATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3155	1987	540	616	12			
1	B	400	Total	C	N	O	S	0	0	0
			3160	1991	542	615	12			
1	C	410	Total	C	N	O	S	0	0	0
			3246	2044	556	634	12			
1	D	402	Total	C	N	O	S	0	0	0
			3175	2000	544	619	12			
1	E	395	Total	C	N	O	S	0	0	0
			3119	1967	534	606	12			
1	F	414	Total	C	N	O	S	0	0	0
			3274	2060	561	640	13			
1	G	414	Total	C	N	O	S	0	0	0
			3278	2062	563	641	12			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP Q8KNP3
B	2	VAL	LEU	engineered mutation	UNP Q8KNP3
C	2	VAL	LEU	engineered mutation	UNP Q8KNP3
D	2	VAL	LEU	engineered mutation	UNP Q8KNP3
E	2	VAL	LEU	engineered mutation	UNP Q8KNP3
F	2	VAL	LEU	engineered mutation	UNP Q8KNP3
G	2	VAL	LEU	engineered mutation	UNP Q8KNP3

- Molecule 2 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

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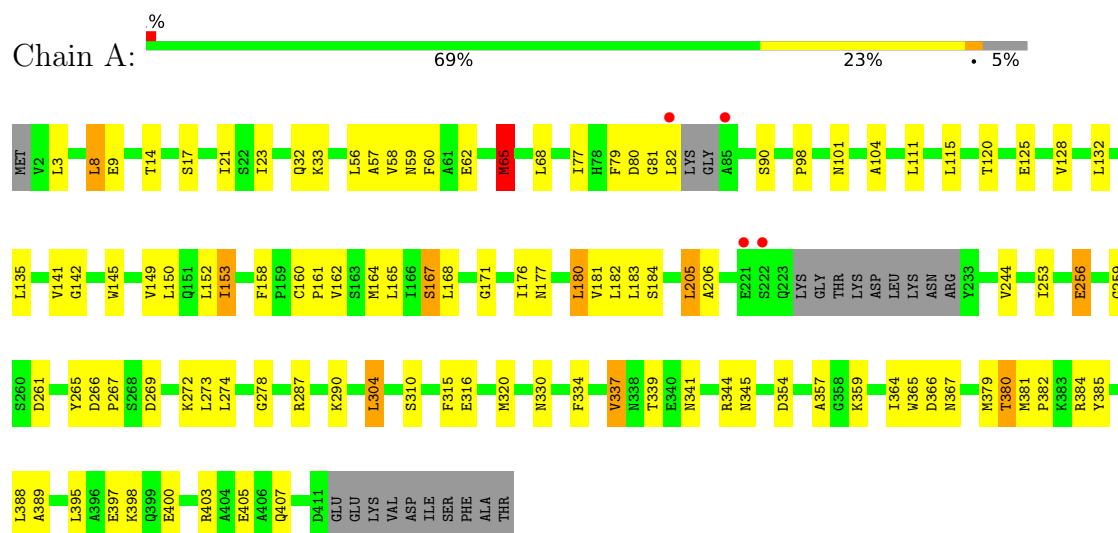
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0

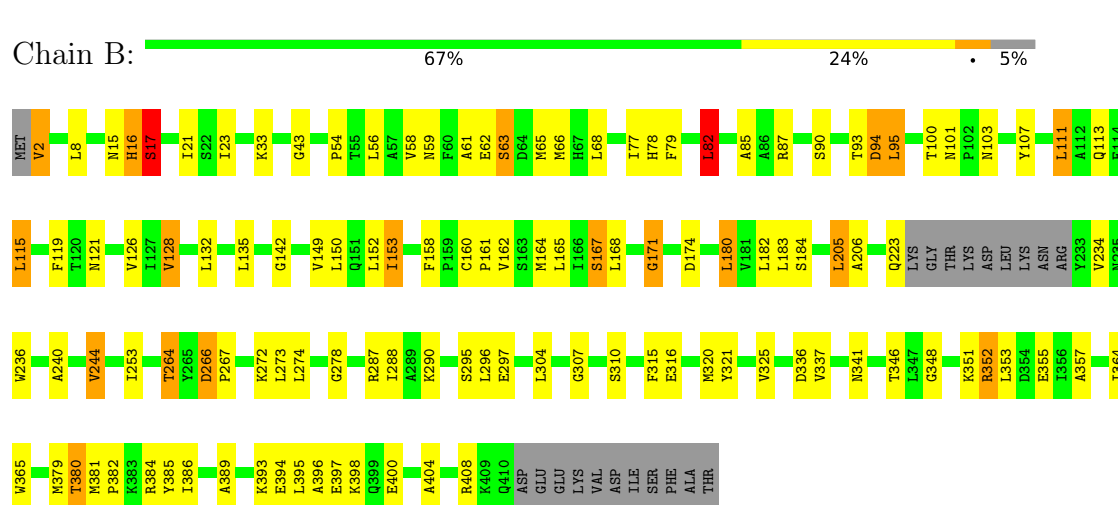
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

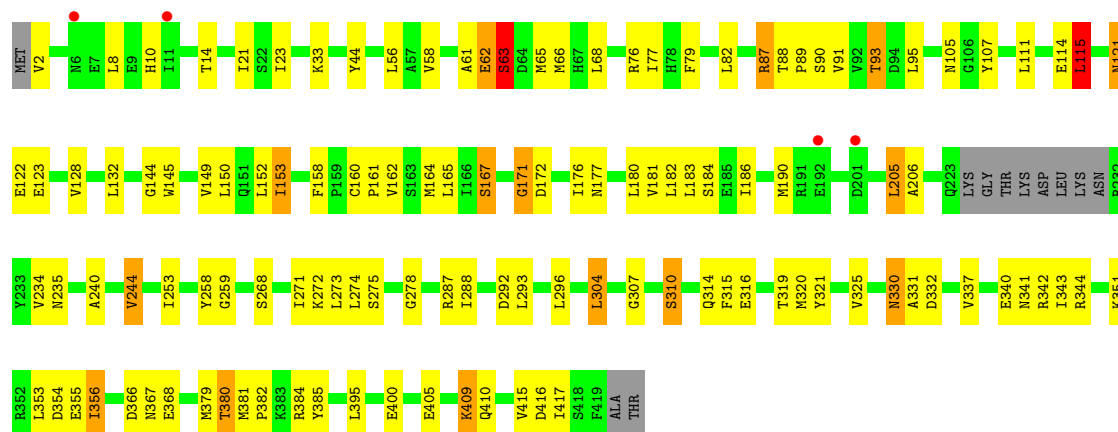


• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN



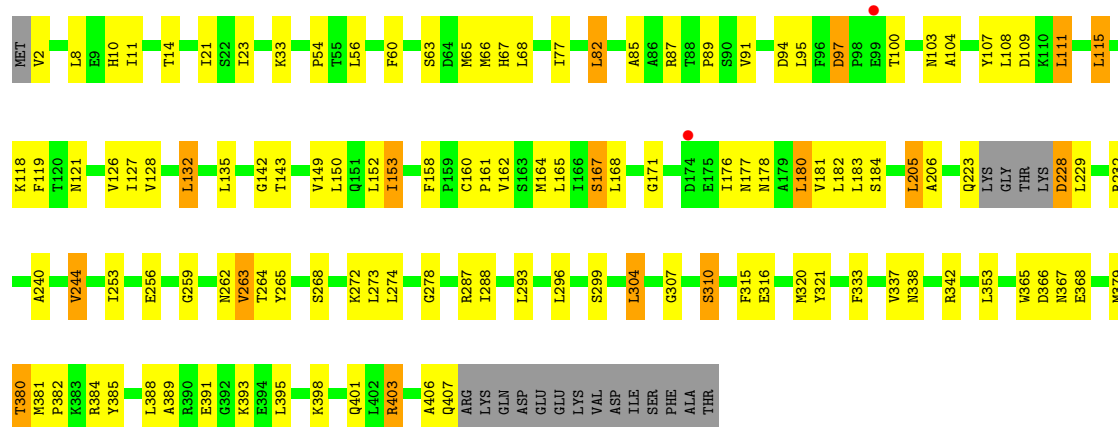
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN





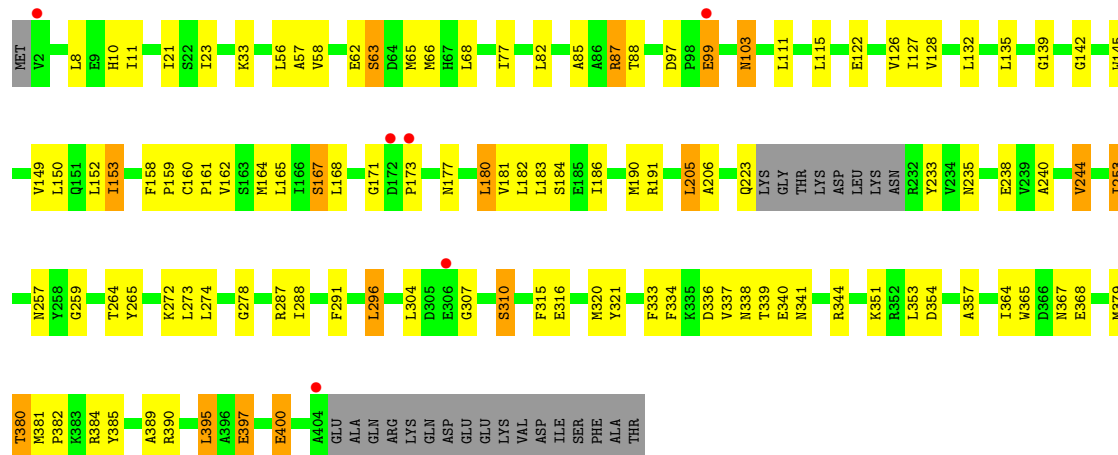
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain D: 67% 25% 5%

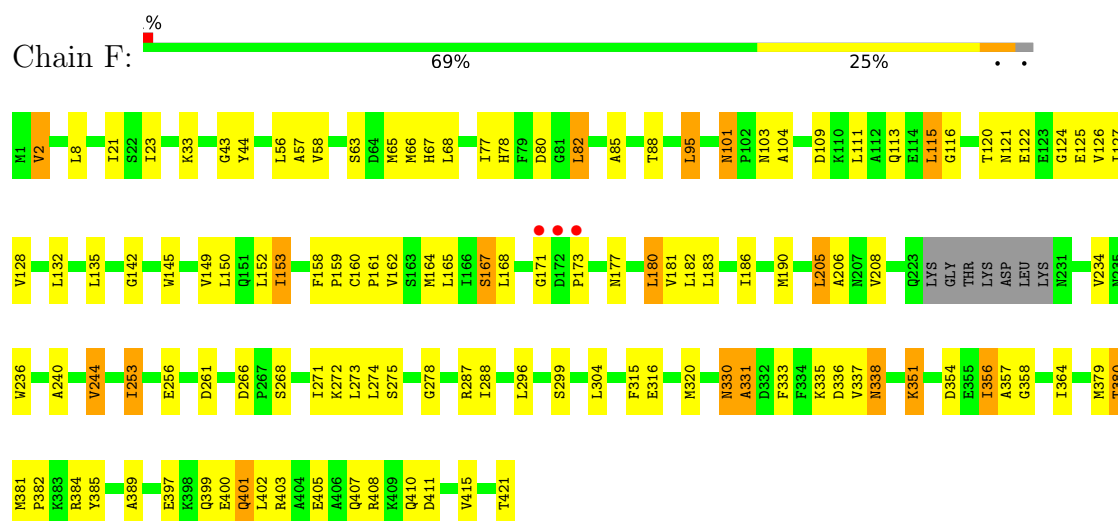


• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

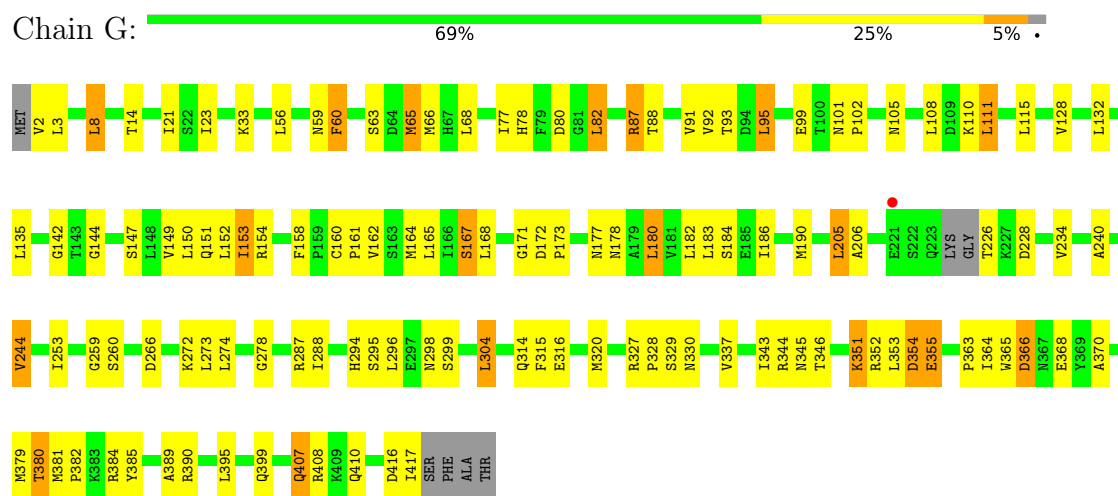
Chain E: 67% 23% 6%



• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN



- Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.06Å 85.15Å 632.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.5 (50.00-3.00) 92.5 (50.00-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.232 , 0.284 (Not available) , 0.240	Depositor DCC
R_{free} test set	2694 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.968	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	22638	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GSP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/3215	0.92	1/4348 (0.0%)
1	B	0.71	0/3221	0.95	5/4356 (0.1%)
1	C	0.73	0/3308	0.91	1/4472 (0.0%)
1	D	0.72	0/3236	0.93	3/4377 (0.1%)
1	E	0.75	0/3180	0.93	1/4302 (0.0%)
1	F	0.76	0/3336	0.95	4/4510 (0.1%)
1	G	0.73	0/3339	0.93	1/4513 (0.0%)
All	All	0.73	0/22835	0.93	16/30878 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	SER	CA-C-N	-7.76	114.35	121.65
1	B	17	SER	C-N-CA	-7.76	114.35	121.65
1	D	97	ASP	CA-C-N	6.74	126.25	119.24
1	D	97	ASP	C-N-CA	6.74	126.25	119.24
1	F	400	GLU	N-CA-C	-6.46	104.32	111.36
1	B	266	ASP	CA-C-N	6.05	126.48	119.47
1	B	266	ASP	C-N-CA	6.05	126.48	119.47
1	E	253	ILE	CB-CA-C	-6.03	104.25	111.97
1	D	229	LEU	N-CA-C	5.89	117.50	111.14
1	F	85	ALA	N-CA-C	-5.89	102.60	110.55
1	F	101	ASN	N-CA-C	5.88	117.08	109.72
1	B	82	LEU	N-CA-C	-5.86	102.75	110.43
1	A	65	MET	N-CA-C	5.75	119.99	112.92
1	C	122	GLU	N-CA-C	-5.35	105.37	111.14
1	F	253	ILE	CB-CA-C	-5.23	105.27	111.97
1	G	60	PHE	N-CA-C	5.17	119.81	112.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3155	0	3064	68	0
1	B	3160	0	3077	90	0
1	C	3246	0	3157	87	0
1	D	3175	0	3090	86	0
1	E	3119	0	3037	83	0
1	F	3274	0	3187	70	0
1	G	3278	0	3197	85	0
2	A	32	0	12	1	0
2	B	32	0	12	2	0
2	C	32	0	12	0	0
2	D	32	0	12	0	0
2	E	32	0	12	1	0
2	F	32	0	12	0	0
2	G	32	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
All	All	22638	0	21893	530	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (530) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:SER:HB2	1:G:66:MET:CE	1.68	1.23
1:G:288:ILE:HD13	1:G:296:LEU:HD12	1.26	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:ILE:HD13	1:D:296:LEU:HD12	1.27	1.14
1:G:288:ILE:HD13	1:G:296:LEU:CD1	1.77	1.12
1:G:63:SER:HB2	1:G:66:MET:HE2	1.09	1.05
1:G:288:ILE:CD1	1:G:296:LEU:HD12	1.90	1.01
1:D:288:ILE:CD1	1:D:296:LEU:HD12	1.92	0.98
1:D:183:LEU:HD22	1:D:381:MET:HE1	1.45	0.98
1:G:63:SER:CB	1:G:66:MET:HE2	1.93	0.97
1:A:341:ASN:HA	1:A:344:ARG:HB3	1.46	0.96
1:G:288:ILE:CD1	1:G:296:LEU:CD1	2.44	0.93
1:E:183:LEU:HD22	1:E:381:MET:HE1	1.51	0.93
1:B:183:LEU:HD22	1:B:381:MET:HE1	1.55	0.87
1:A:183:LEU:HD22	1:A:381:MET:HE1	1.55	0.87
1:G:183:LEU:HD22	1:G:381:MET:HE1	1.56	0.87
1:C:183:LEU:HD22	1:C:381:MET:HE1	1.58	0.86
1:E:288:ILE:CD1	1:E:296:LEU:HD12	2.06	0.84
1:B:95:LEU:HD21	1:B:107:TYR:CG	2.11	0.84
1:B:288:ILE:CD1	1:B:296:LEU:HD12	2.08	0.84
1:B:2:VAL:HG21	1:B:43:GLY:C	2.02	0.83
1:C:355:GLU:O	1:C:356:ILE:HG23	1.77	0.83
1:F:357:ALA:HA	1:G:172:ASP:OD2	1.79	0.83
1:A:58:VAL:HG11	1:A:145:TRP:CZ2	2.13	0.83
1:G:23:ILE:HD12	1:G:274:LEU:HD12	1.60	0.82
1:F:23:ILE:HD12	1:F:274:LEU:HD12	1.60	0.82
1:B:288:ILE:HD13	1:B:296:LEU:HD12	1.61	0.81
1:E:23:ILE:HD12	1:E:274:LEU:HD12	1.62	0.81
1:C:82:LEU:HD11	1:C:91:VAL:HG12	1.63	0.81
1:F:183:LEU:HD22	1:F:381:MET:HE1	1.63	0.81
1:B:82:LEU:HD12	1:B:82:LEU:H	1.44	0.80
1:A:23:ILE:HD12	1:A:274:LEU:HD12	1.64	0.80
1:D:268:SER:OG	1:E:85:ALA:O	2.01	0.79
1:B:400:GLU:O	1:B:404:ALA:HB2	1.83	0.79
1:D:23:ILE:HD12	1:D:274:LEU:HD12	1.64	0.79
1:B:15:ASN:OD1	1:B:17:SER:N	2.16	0.79
1:B:126:VAL:HG12	1:B:128:VAL:H	1.48	0.78
1:G:63:SER:O	1:G:66:MET:HG2	1.84	0.77
1:C:23:ILE:HD12	1:C:274:LEU:HD12	1.67	0.77
1:F:116:GLY:O	1:F:120:THR:OG1	2.03	0.76
1:A:81:GLY:O	1:A:82:LEU:HD23	1.87	0.75
1:A:3:LEU:HD13	1:A:9:GLU:HA	1.69	0.75
1:E:63:SER:HA	1:E:66:MET:HE2	1.67	0.74
1:G:288:ILE:HB	1:G:370:ALA:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ILE:HD12	1:B:274:LEU:HD12	1.69	0.74
1:F:288:ILE:HD13	1:F:296:LEU:HD12	1.70	0.74
1:A:58:VAL:C	1:A:65:MET:HE1	2.14	0.73
1:B:95:LEU:HD11	1:B:107:TYR:CZ	2.22	0.73
1:C:149:VAL:HG11	1:C:164:MET:HE3	1.69	0.73
1:C:82:LEU:CD1	1:C:91:VAL:HG12	2.19	0.72
1:D:288:ILE:HD13	1:D:296:LEU:CD1	2.16	0.72
1:E:57:ALA:O	1:E:65:MET:HE1	1.89	0.71
1:B:95:LEU:C	1:B:95:LEU:HD23	2.16	0.71
1:E:259:GLY:HA3	1:F:66:MET:HE3	1.71	0.70
1:D:63:SER:CB	1:D:66:MET:HE2	2.19	0.70
1:C:259:GLY:CA	1:D:66:MET:HE3	2.22	0.69
1:A:357:ALA:HB2	1:B:174:ASP:OD1	1.92	0.69
1:C:77:ILE:HG22	1:C:79:PHE:CE2	2.27	0.69
1:D:259:GLY:N	1:E:66:MET:HE3	2.07	0.69
1:E:57:ALA:CB	1:E:65:MET:HE2	2.23	0.69
1:F:315:PHE:HA	1:F:379:MET:HE2	1.74	0.68
1:C:315:PHE:HA	1:C:379:MET:HE2	1.74	0.68
1:B:315:PHE:HA	1:B:379:MET:HE2	1.75	0.68
1:A:141:VAL:HG23	2:A:900:GSP:S1G	2.34	0.68
1:D:228:ASP:OD2	1:D:228:ASP:C	2.37	0.68
1:G:288:ILE:HD13	1:G:296:LEU:HD13	1.73	0.68
1:C:259:GLY:N	1:D:66:MET:HE3	2.08	0.68
1:G:149:VAL:HG11	1:G:164:MET:HE3	1.76	0.68
1:B:77:ILE:HG22	1:B:79:PHE:CE2	2.29	0.68
1:B:149:VAL:HG11	1:B:164:MET:HE3	1.75	0.67
1:D:315:PHE:HA	1:D:379:MET:HE2	1.76	0.67
1:E:288:ILE:HD13	1:E:296:LEU:HD12	1.74	0.67
1:C:149:VAL:CG1	1:C:164:MET:HE3	2.24	0.67
1:D:391:GLU:O	1:D:395:LEU:HD23	1.95	0.66
1:D:288:ILE:CD1	1:D:296:LEU:CD1	2.70	0.66
1:F:288:ILE:CD1	1:F:296:LEU:HD12	2.26	0.66
1:A:381:MET:HE3	1:A:382:PRO:HD2	1.77	0.66
1:G:56:LEU:HD22	1:G:77:ILE:CD1	2.25	0.66
1:G:381:MET:HE3	1:G:382:PRO:HD2	1.75	0.66
1:B:393:LYS:HD3	1:C:417:ILE:HG23	1.78	0.66
1:G:60:PHE:O	1:G:78:HIS:CD2	2.48	0.66
1:A:58:VAL:HG11	1:A:145:TRP:CE2	2.31	0.65
1:C:341:ASN:HA	1:C:344:ARG:HB3	1.78	0.65
1:G:272:LYS:HG2	1:G:320:MET:HE1	1.78	0.65
1:C:63:SER:HA	1:C:66:MET:HE2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:381:MET:HE2	1:E:385:TYR:HB2	1.79	0.64
1:B:381:MET:HE3	1:B:382:PRO:HD2	1.80	0.64
1:B:111:LEU:HD22	1:B:115:LEU:HD22	1.79	0.64
1:D:272:LYS:HG2	1:D:320:MET:HE1	1.80	0.64
1:E:381:MET:HE3	1:E:382:PRO:HD2	1.78	0.64
1:G:328:PRO:HA	1:G:365:TRP:O	1.98	0.64
1:G:351:LYS:NZ	1:G:355:GLU:OE2	2.27	0.64
1:D:149:VAL:HG11	1:D:164:MET:HE3	1.80	0.63
1:G:65:MET:HE1	1:G:77:ILE:O	1.99	0.63
1:C:288:ILE:HD13	1:C:296:LEU:HD12	1.80	0.63
1:D:63:SER:HB2	1:D:66:MET:HE2	1.79	0.62
1:E:315:PHE:HA	1:E:379:MET:HE2	1.80	0.62
1:E:58:VAL:HG11	1:E:145:TRP:CH2	2.33	0.62
1:F:177:ASN:O	1:F:181:VAL:HG13	1.99	0.62
1:G:56:LEU:HD22	1:G:77:ILE:HD11	1.81	0.62
1:C:288:ILE:CD1	1:C:296:LEU:HD12	2.30	0.62
1:D:56:LEU:HD22	1:D:77:ILE:CD1	2.29	0.62
1:G:149:VAL:CG1	1:G:164:MET:HE3	2.30	0.62
1:F:358:GLY:N	1:G:172:ASP:OD2	2.30	0.62
1:G:381:MET:HE2	1:G:385:TYR:HB2	1.81	0.62
1:D:21:ILE:HG22	1:D:253:ILE:HD13	1.82	0.62
1:D:2:VAL:HG23	1:D:2:VAL:O	1.99	0.61
1:F:381:MET:HE3	1:F:382:PRO:HD2	1.81	0.61
1:A:272:LYS:HG2	1:A:320:MET:HE1	1.81	0.61
1:A:149:VAL:HG11	1:A:164:MET:HE3	1.82	0.61
1:C:272:LYS:HG2	1:C:320:MET:HE1	1.82	0.61
1:D:23:ILE:CD1	1:D:274:LEU:HD12	2.31	0.61
1:C:56:LEU:HD22	1:C:77:ILE:CD1	2.31	0.61
1:F:381:MET:HE2	1:F:385:TYR:HB2	1.82	0.61
1:F:23:ILE:CD1	1:F:274:LEU:HD12	2.30	0.60
1:D:262:ASN:ND2	1:D:263:VAL:HG23	2.15	0.60
1:F:122:GLU:OE2	1:F:122:GLU:HA	2.01	0.60
1:G:78:HIS:O	1:G:110:LYS:NZ	2.34	0.60
1:E:259:GLY:CA	1:F:66:MET:HE3	2.31	0.60
1:A:176:ILE:HG23	1:A:388:LEU:HD22	1.82	0.60
1:B:56:LEU:HD22	1:B:77:ILE:CD1	2.31	0.60
1:G:63:SER:HB2	1:G:66:MET:HE1	1.74	0.60
1:B:149:VAL:CG1	1:B:164:MET:HE3	2.31	0.60
1:D:381:MET:HE2	1:D:385:TYR:HB2	1.84	0.60
1:E:272:LYS:HG2	1:E:320:MET:HE1	1.84	0.60
1:E:57:ALA:HB1	1:E:65:MET:HE2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:PHE:HA	1:G:379:MET:HE2	1.82	0.60
1:A:21:ILE:HG22	1:A:253:ILE:HD13	1.84	0.59
1:D:54:PRO:HB2	1:D:119:PHE:CE2	2.37	0.59
1:G:23:ILE:CD1	1:G:274:LEU:HD12	2.31	0.59
1:B:126:VAL:HG12	1:B:128:VAL:N	2.17	0.59
1:D:381:MET:HE3	1:D:382:PRO:HD2	1.83	0.59
1:B:21:ILE:HG22	1:B:253:ILE:HD13	1.84	0.59
1:C:56:LEU:HD22	1:C:77:ILE:HD11	1.83	0.59
1:A:23:ILE:CD1	1:A:274:LEU:HD12	2.31	0.59
1:E:149:VAL:HG11	1:E:164:MET:HE3	1.85	0.59
1:E:23:ILE:CD1	1:E:274:LEU:HD12	2.32	0.59
1:E:321:TYR:CE1	1:E:353:LEU:HD13	2.37	0.59
1:F:56:LEU:HD22	1:F:77:ILE:CD1	2.32	0.59
1:E:337:VAL:HG23	1:F:234:VAL:O	2.03	0.59
1:C:381:MET:HE3	1:C:382:PRO:HD2	1.84	0.58
1:B:272:LYS:HG2	1:B:320:MET:HE1	1.85	0.58
1:D:259:GLY:CA	1:E:66:MET:HE3	2.32	0.58
1:F:272:LYS:HG2	1:F:320:MET:HE1	1.84	0.58
1:A:315:PHE:HA	1:A:379:MET:HE2	1.85	0.58
1:D:56:LEU:HD22	1:D:77:ILE:HD11	1.84	0.58
1:D:259:GLY:HA3	1:E:66:MET:HE3	1.85	0.58
1:F:149:VAL:HG11	1:F:164:MET:HE3	1.85	0.58
1:B:56:LEU:HD22	1:B:77:ILE:HD11	1.86	0.58
1:E:56:LEU:HD22	1:E:77:ILE:CD1	2.34	0.58
1:F:153:ILE:HG22	1:F:158:PHE:CD1	2.39	0.58
1:C:258:TYR:C	1:D:66:MET:HE3	2.29	0.57
1:F:56:LEU:HD22	1:F:77:ILE:HD11	1.84	0.57
1:G:93:THR:HG22	1:G:144:GLY:O	2.04	0.57
1:E:153:ILE:HG22	1:E:158:PHE:CD1	2.39	0.57
1:G:228:ASP:OD2	1:G:228:ASP:C	2.47	0.57
1:B:23:ILE:CD1	1:B:274:LEU:HD12	2.35	0.57
1:C:153:ILE:HG22	1:C:158:PHE:CD1	2.39	0.57
1:C:381:MET:HE2	1:C:385:TYR:HB2	1.85	0.57
1:E:57:ALA:C	1:E:65:MET:CE	2.78	0.57
1:G:206:ALA:O	1:G:278:GLY:HA2	2.05	0.57
1:C:65:MET:HE1	1:C:77:ILE:N	2.21	0.56
1:A:56:LEU:HD22	1:A:77:ILE:CD1	2.35	0.56
1:C:23:ILE:CD1	1:C:274:LEU:HD12	2.35	0.56
1:D:153:ILE:HG22	1:D:158:PHE:CD1	2.41	0.56
1:F:401:GLN:HG2	1:F:402:LEU:N	2.20	0.56
1:D:149:VAL:CG1	1:D:164:MET:HE3	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASN:HB3	1:B:65:MET:HE2	1.87	0.56
1:A:176:ILE:CG2	1:A:388:LEU:HD22	2.36	0.56
1:B:381:MET:HB3	1:C:410:GLN:HE22	1.71	0.56
1:E:177:ASN:O	1:E:181:VAL:HG13	2.06	0.56
1:B:381:MET:HE2	1:B:385:TYR:HB2	1.86	0.56
1:C:21:ILE:HG22	1:C:253:ILE:HD13	1.87	0.55
1:C:61:ALA:HB2	1:C:87:ARG:NH1	2.21	0.55
1:F:21:ILE:HG22	1:F:253:ILE:HD13	1.87	0.55
1:A:149:VAL:CG1	1:A:164:MET:HE3	2.36	0.55
1:C:77:ILE:CG2	1:C:79:PHE:CE2	2.89	0.55
1:G:82:LEU:HD13	1:G:95:LEU:HD22	1.88	0.55
1:A:381:MET:HE2	1:A:385:TYR:HB2	1.86	0.55
1:E:57:ALA:C	1:E:65:MET:HE1	2.31	0.55
1:E:103:ASN:N	1:E:103:ASN:OD1	2.39	0.55
1:A:59:ASN:HB2	1:A:65:MET:HE3	1.88	0.54
1:A:56:LEU:HD22	1:A:77:ILE:HD11	1.89	0.54
1:B:160:CYS:HB2	1:B:161:PRO:CD	2.37	0.54
1:A:21:ILE:C	1:A:256:GLU:HG3	2.31	0.54
1:B:320:MET:HG3	1:B:357:ALA:HB3	1.90	0.54
1:C:90:SER:HA	1:C:93:THR:HG23	1.89	0.54
1:F:330:ASN:CG	1:F:331:ALA:N	2.64	0.54
1:G:173:PRO:HB3	1:G:395:LEU:HD12	1.89	0.54
1:F:271:ILE:O	1:F:275:SER:OG	2.23	0.54
1:G:329:SER:HA	1:G:364:ILE:HG21	1.90	0.54
1:A:160:CYS:HB2	1:A:161:PRO:CD	2.38	0.54
1:A:58:VAL:CA	1:A:65:MET:HE1	2.37	0.54
1:C:206:ALA:O	1:C:278:GLY:HA2	2.08	0.54
1:C:65:MET:HE2	1:C:76:ARG:HB3	1.89	0.54
1:D:91:VAL:HG12	1:D:91:VAL:O	2.07	0.54
1:A:153:ILE:HG22	1:A:158:PHE:CD1	2.43	0.53
1:D:380:THR:HG23	1:D:381:MET:N	2.23	0.53
1:B:95:LEU:HD11	1:B:107:TYR:CE2	2.43	0.53
1:D:11:ILE:HG22	1:D:365:TRP:HE3	1.73	0.53
1:E:56:LEU:HD22	1:E:77:ILE:HD11	1.89	0.53
1:A:359:LYS:NZ	2:B:900:GSP:O3G	2.41	0.53
1:F:149:VAL:CG1	1:F:164:MET:HE3	2.38	0.53
1:D:183:LEU:CD2	1:D:381:MET:HE1	2.30	0.53
1:E:87:ARG:NH2	2:E:900:GSP:O2G	2.42	0.53
1:D:160:CYS:HB2	1:D:161:PRO:CD	2.39	0.53
1:F:160:CYS:HB2	1:F:161:PRO:CD	2.39	0.53
1:D:111:LEU:HD22	1:D:115:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:ASN:O	1:D:181:VAL:HG13	2.09	0.53
1:B:397:GLU:O	1:B:398:LYS:C	2.52	0.52
1:D:14:THR:CG2	1:D:366:ASP:HB2	2.39	0.52
1:G:101:ASN:OD1	1:G:101:ASN:C	2.52	0.52
1:G:160:CYS:HB2	1:G:161:PRO:CD	2.39	0.52
1:G:353:LEU:HD23	1:G:353:LEU:N	2.22	0.52
1:B:62:GLU:OE2	1:B:78:HIS:CB	2.58	0.52
1:F:357:ALA:CA	1:G:172:ASP:OD2	2.54	0.52
1:B:153:ILE:HG22	1:B:158:PHE:CD1	2.45	0.52
1:B:240:ALA:O	1:B:244:VAL:HG13	2.09	0.52
1:F:336:ASP:OD1	1:F:338:ASN:HB2	2.09	0.52
1:G:153:ILE:HG22	1:G:158:PHE:CD1	2.45	0.52
1:A:334:PHE:HA	1:A:339:THR:HG21	1.92	0.52
1:B:61:ALA:HB2	1:B:87:ARG:NH2	2.25	0.52
1:E:206:ALA:O	1:E:278:GLY:HA2	2.10	0.51
1:E:337:VAL:HG22	1:F:236:TRP:HB3	1.92	0.51
1:E:288:ILE:HD11	1:E:296:LEU:HD12	1.89	0.51
1:E:149:VAL:CG1	1:E:164:MET:HE3	2.40	0.51
1:E:364:ILE:HD12	1:F:67:HIS:CE1	2.45	0.51
1:C:2:VAL:HG23	1:C:44:TYR:CD1	2.45	0.51
1:D:264:THR:HG21	1:E:63:SER:HB2	1.92	0.51
1:E:126:VAL:HG21	1:E:159:PRO:CB	2.41	0.51
1:F:380:THR:HG23	1:F:381:MET:N	2.25	0.51
1:G:21:ILE:HG22	1:G:253:ILE:HD13	1.92	0.51
1:G:135:LEU:HD22	1:G:142:GLY:O	2.11	0.51
1:E:173:PRO:HG3	1:E:395:LEU:HD22	1.93	0.51
1:G:162:VAL:O	1:G:205:LEU:HD23	2.10	0.51
1:A:357:ALA:CB	1:B:174:ASP:OD1	2.58	0.51
1:C:160:CYS:HB2	1:C:161:PRO:CD	2.41	0.51
1:C:177:ASN:O	1:C:181:VAL:HG13	2.11	0.51
1:A:98:PRO:HA	1:A:101:ASN:O	2.11	0.51
1:F:261:ASP:OD2	1:F:364:ILE:HD11	2.11	0.51
1:B:62:GLU:OE2	1:B:78:HIS:HB2	2.10	0.51
1:F:135:LEU:HD22	1:F:142:GLY:O	2.11	0.51
1:B:162:VAL:O	1:B:205:LEU:HD23	2.11	0.50
1:E:397:GLU:HA	1:E:400:GLU:HB2	1.93	0.50
1:G:206:ALA:HB1	1:G:274:LEU:O	2.11	0.50
1:C:206:ALA:HB1	1:C:274:LEU:O	2.11	0.50
1:C:315:PHE:CD2	1:C:379:MET:CE	2.94	0.50
1:E:240:ALA:O	1:E:244:VAL:HG13	2.11	0.50
1:D:10:HIS:HB3	1:D:367:ASN:CG	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:ILE:CG2	1:E:365:TRP:HZ3	2.25	0.50
1:B:355:GLU:CB	1:C:395:LEU:HD22	2.41	0.50
1:B:380:THR:HG23	1:B:381:MET:N	2.26	0.50
1:E:173:PRO:O	1:E:177:ASN:CG	2.55	0.50
1:A:168:LEU:HD21	1:A:183:LEU:HD11	1.93	0.50
1:B:364:ILE:HG22	1:B:365:TRP:N	2.26	0.50
1:F:2:VAL:HG23	1:F:44:TYR:CD1	2.46	0.50
1:B:297:GLU:HG3	1:B:346:THR:OG1	2.11	0.50
1:G:82:LEU:HD23	1:G:87:ARG:HG3	1.94	0.50
1:A:162:VAL:O	1:A:205:LEU:HD23	2.11	0.50
1:C:319:THR:HA	1:C:356:ILE:HG21	1.94	0.50
1:G:56:LEU:HD22	1:G:77:ILE:HD12	1.93	0.50
1:C:93:THR:HG22	1:C:144:GLY:CA	2.41	0.50
1:A:206:ALA:O	1:A:278:GLY:HA2	2.12	0.49
1:D:337:VAL:HG23	1:D:338:ASN:OD1	2.12	0.49
1:A:79:PHE:O	1:A:80:ASP:C	2.55	0.49
1:B:82:LEU:HD22	1:B:85:ALA:CB	2.42	0.49
1:B:364:ILE:CG2	1:B:365:TRP:N	2.75	0.49
1:E:21:ILE:HG22	1:E:253:ILE:HD13	1.94	0.49
1:E:11:ILE:CG2	1:E:365:TRP:CZ3	2.96	0.49
1:E:57:ALA:HB3	1:E:65:MET:HE2	1.95	0.49
1:A:57:ALA:HB1	1:A:65:MET:HE2	1.94	0.49
1:A:315:PHE:CD2	1:A:379:MET:CE	2.96	0.49
1:B:21:ILE:HD12	1:B:23:ILE:O	2.12	0.49
1:B:160:CYS:HB2	1:B:161:PRO:HD2	1.94	0.49
1:C:33:LYS:HE3	1:C:167:SER:HB3	1.95	0.49
1:D:206:ALA:O	1:D:278:GLY:HA2	2.13	0.49
1:E:160:CYS:HB2	1:E:161:PRO:CD	2.42	0.49
1:G:110:LYS:O	1:G:111:LEU:C	2.54	0.49
1:G:186:ILE:CG2	1:G:190:MET:HE3	2.42	0.49
1:G:288:ILE:HD11	1:G:296:LEU:HD12	1.88	0.49
1:F:2:VAL:HG22	1:F:43:GLY:HA3	1.94	0.49
1:F:357:ALA:HA	1:G:172:ASP:CG	2.37	0.49
1:C:121:ASN:HB3	1:C:123:GLU:N	2.27	0.49
1:C:380:THR:HG23	1:C:381:MET:N	2.27	0.49
1:E:10:HIS:HB3	1:E:367:ASN:ND2	2.28	0.49
1:B:33:LYS:HE3	1:B:167:SER:HB3	1.95	0.49
1:A:98:PRO:HG3	1:A:104:ALA:HB3	1.94	0.48
1:E:320:MET:HG3	1:E:357:ALA:O	2.13	0.48
1:G:353:LEU:O	1:G:354:ASP:C	2.56	0.48
1:B:266:ASP:HB2	1:B:267:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:VAL:O	1:C:205:LEU:HD23	2.13	0.48
1:B:100:THR:HG22	1:B:101:ASN:N	2.29	0.48
1:D:293:LEU:HD13	1:D:342:ARG:HB2	1.96	0.48
1:G:168:LEU:HD21	1:G:183:LEU:HD11	1.95	0.48
1:G:343:ILE:O	1:G:346:THR:N	2.47	0.48
1:E:338:ASN:O	1:E:339:THR:C	2.56	0.48
1:B:315:PHE:CD2	1:B:379:MET:CE	2.97	0.48
1:D:14:THR:HG21	1:D:366:ASP:HB2	1.96	0.48
1:E:334:PHE:HA	1:E:339:THR:HG21	1.96	0.48
1:F:57:ALA:O	1:F:65:MET:HE1	2.13	0.48
1:C:58:VAL:HG11	1:C:145:TRP:CH2	2.49	0.48
1:G:272:LYS:CG	1:G:320:MET:HE1	2.44	0.48
1:A:354:ASP:HA	1:B:171:GLY:O	2.14	0.48
1:F:315:PHE:CD2	1:F:379:MET:CE	2.96	0.48
1:F:320:MET:HG3	1:F:357:ALA:O	2.13	0.48
1:C:171:GLY:HA2	1:C:176:ILE:HD11	1.96	0.48
1:D:162:VAL:O	1:D:205:LEU:HD23	2.13	0.48
1:G:63:SER:O	1:G:66:MET:HE2	2.14	0.48
1:C:315:PHE:CD2	1:C:379:MET:HE1	2.48	0.48
1:D:95:LEU:HD11	1:D:107:TYR:CE1	2.49	0.47
1:D:183:LEU:HD22	1:D:381:MET:CE	2.32	0.47
1:C:330:ASN:O	1:C:332:ASP:N	2.45	0.47
1:D:264:THR:HG22	1:D:265:TYR:O	2.14	0.47
1:G:111:LEU:HD23	1:G:115:LEU:HD13	1.96	0.47
1:E:33:LYS:HE3	1:E:167:SER:HB3	1.96	0.47
1:F:33:LYS:HE3	1:F:167:SER:CB	2.44	0.47
1:F:402:LEU:HA	1:F:405:GLU:HB2	1.95	0.47
1:G:343:ILE:O	1:G:344:ARG:C	2.57	0.47
1:B:206:ALA:HB1	1:B:274:LEU:O	2.14	0.47
1:E:33:LYS:HE3	1:E:167:SER:CB	2.44	0.47
1:E:168:LEU:HD21	1:E:183:LEU:HD11	1.95	0.47
1:F:121:ASN:HB2	1:F:125:GLU:O	2.13	0.47
1:G:3:LEU:HD22	1:G:8:LEU:HB3	1.95	0.47
1:A:33:LYS:HE3	1:A:167:SER:HB3	1.96	0.47
1:C:307:GLY:O	1:C:310:SER:OG	2.32	0.47
1:G:105:ASN:HA	1:G:108:LEU:HB2	1.97	0.47
1:B:206:ALA:O	1:B:278:GLY:HA2	2.14	0.47
1:G:329:SER:HA	1:G:364:ILE:CG2	2.44	0.47
1:B:33:LYS:HE3	1:B:167:SER:CB	2.44	0.47
1:B:54:PRO:HB2	1:B:119:PHE:CE2	2.50	0.47
1:C:95:LEU:HD23	1:C:95:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:PHE:CD2	1:D:379:MET:CE	2.98	0.47
1:E:259:GLY:N	1:F:66:MET:HE3	2.30	0.47
1:G:33:LYS:HE3	1:G:167:SER:HB3	1.97	0.47
1:F:160:CYS:HB2	1:F:161:PRO:HD2	1.97	0.47
1:G:14:THR:HG21	1:G:366:ASP:OD2	2.14	0.47
1:A:33:LYS:HE3	1:A:167:SER:CB	2.45	0.47
1:A:380:THR:HG23	1:A:381:MET:N	2.30	0.46
1:F:33:LYS:HE3	1:F:167:SER:HB3	1.97	0.46
1:G:407:GLN:O	1:G:408:ARG:C	2.58	0.46
1:A:180:LEU:HD21	1:A:389:ALA:HA	1.97	0.46
1:F:168:LEU:HD21	1:F:183:LEU:HD11	1.98	0.46
1:B:307:GLY:O	1:B:310:SER:OG	2.34	0.46
1:E:87:ARG:HD2	1:E:139:GLY:HA2	1.97	0.46
1:E:291:PHE:HB3	1:E:333:PHE:CD2	2.51	0.46
1:B:95:LEU:HD21	1:B:107:TYR:CD1	2.50	0.46
1:D:54:PRO:HB2	1:D:119:PHE:HE2	1.80	0.46
1:B:321:TYR:CG	1:B:353:LEU:HD22	2.51	0.46
1:G:160:CYS:HB2	1:G:161:PRO:HD2	1.98	0.46
1:C:115:LEU:HD12	1:C:115:LEU:HA	1.65	0.46
1:C:160:CYS:HB2	1:C:161:PRO:HD2	1.98	0.46
1:F:101:ASN:O	1:F:104:ALA:HB2	2.16	0.46
1:C:354:ASP:HB2	1:D:398:LYS:HZ1	1.80	0.46
1:D:2:VAL:O	1:D:2:VAL:CG2	2.63	0.46
1:D:160:CYS:HB2	1:D:161:PRO:HD2	1.97	0.46
1:E:272:LYS:CG	1:E:320:MET:HE1	2.45	0.46
1:C:88:THR:HB	1:C:89:PRO:HD2	1.97	0.45
1:E:341:ASN:HA	1:E:344:ARG:HB3	1.98	0.45
1:F:162:VAL:O	1:F:205:LEU:HD23	2.15	0.45
1:B:95:LEU:HD21	1:B:107:TYR:CD2	2.49	0.45
1:C:33:LYS:HE3	1:C:167:SER:CB	2.45	0.45
1:C:271:ILE:O	1:C:275:SER:OG	2.35	0.45
1:C:272:LYS:CG	1:C:320:MET:HE1	2.46	0.45
1:B:62:GLU:HG2	1:B:78:HIS:CD2	2.51	0.45
1:D:240:ALA:O	1:D:244:VAL:HG13	2.17	0.45
1:C:82:LEU:CD1	1:C:91:VAL:CG1	2.91	0.45
1:D:85:ALA:HB1	1:D:91:VAL:HB	1.99	0.45
1:A:177:ASN:O	1:A:181:VAL:HG13	2.17	0.45
1:C:321:TYR:CZ	1:C:353:LEU:HD23	2.52	0.45
1:E:315:PHE:CD2	1:E:379:MET:CE	3.00	0.45
1:F:126:VAL:HG21	1:F:159:PRO:CB	2.47	0.45
1:A:315:PHE:CD2	1:A:379:MET:HE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:PHE:CD2	1:F:379:MET:HE1	2.52	0.45
1:C:121:ASN:HB3	1:C:123:GLU:H	1.82	0.45
1:D:168:LEU:HD21	1:D:183:LEU:HD11	1.99	0.45
1:E:380:THR:HG23	1:E:381:MET:N	2.32	0.45
1:E:354:ASP:O	1:F:173:PRO:HD3	2.17	0.45
1:A:160:CYS:HB2	1:A:161:PRO:HD2	1.98	0.45
1:C:82:LEU:HG	1:C:95:LEU:HD12	1.97	0.45
1:E:180:LEU:HD21	1:E:389:ALA:HA	1.99	0.45
1:B:56:LEU:HD22	1:B:77:ILE:HD12	2.00	0.45
1:E:11:ILE:HG22	1:E:365:TRP:CE3	2.52	0.44
1:E:97:ASP:OD1	1:E:99:GLU:HB3	2.17	0.44
1:B:386:ILE:HD11	1:C:409:LYS:NZ	2.32	0.44
1:D:33:LYS:HE3	1:D:167:SER:HB3	2.00	0.44
1:E:56:LEU:CD1	1:E:115:LEU:HD12	2.47	0.44
1:F:63:SER:CB	1:F:66:MET:HE2	2.47	0.44
1:F:351:LYS:HD2	1:F:356:ILE:HD13	1.99	0.44
1:A:59:ASN:N	1:A:65:MET:HE1	2.32	0.44
1:A:315:PHE:HA	1:A:379:MET:CE	2.47	0.44
1:B:357:ALA:HA	1:C:172:ASP:OD2	2.17	0.44
1:A:60:PHE:CZ	1:A:81:GLY:HA3	2.52	0.44
1:A:183:LEU:CD2	1:A:381:MET:HE1	2.38	0.44
1:B:168:LEU:HD21	1:B:183:LEU:HD11	1.98	0.44
1:E:191:ARG:NH1	1:F:410:GLN:C	2.75	0.44
1:E:264:THR:HG22	1:E:265:TYR:N	2.32	0.44
1:G:33:LYS:HE3	1:G:167:SER:CB	2.47	0.44
1:A:59:ASN:HB2	1:A:65:MET:CE	2.47	0.44
1:A:135:LEU:HD22	1:A:142:GLY:O	2.18	0.44
1:A:261:ASP:OD2	1:A:364:ILE:HD11	2.17	0.44
1:A:337:VAL:CG1	1:B:236:TRP:HB3	2.48	0.44
1:C:293:LEU:HD22	1:C:342:ARG:HG2	1.99	0.44
1:D:60:PHE:CD1	1:D:82:LEU:CD2	3.00	0.44
1:C:14:THR:CG2	1:C:366:ASP:HB2	2.47	0.44
1:C:314:GLN:OE1	1:C:380:THR:CG2	2.66	0.44
1:D:33:LYS:HE3	1:D:167:SER:CB	2.48	0.44
1:D:56:LEU:HD22	1:D:77:ILE:HD12	1.97	0.44
1:G:59:ASN:N	1:G:65:MET:HE3	2.32	0.44
1:G:330:ASN:OD1	1:G:330:ASN:C	2.60	0.44
1:B:58:VAL:HG13	1:B:79:PHE:CE2	2.53	0.44
1:C:342:ARG:O	1:C:343:ILE:C	2.60	0.44
1:E:135:LEU:HD22	1:E:142:GLY:O	2.18	0.44
1:E:307:GLY:O	1:E:310:SER:OG	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:PRO:HB3	1:E:395:LEU:HD13	1.99	0.44
1:C:259:GLY:C	1:D:67:HIS:CD2	2.96	0.43
1:D:180:LEU:HD21	1:D:389:ALA:HA	2.00	0.43
1:F:115:LEU:HD12	1:F:115:LEU:HA	1.85	0.43
1:G:180:LEU:HD21	1:G:389:ALA:HA	2.00	0.43
1:D:206:ALA:HB1	1:D:274:LEU:O	2.17	0.43
1:F:121:ASN:HB3	1:F:124:GLY:H	1.84	0.43
1:D:11:ILE:HG22	1:D:365:TRP:CE3	2.52	0.43
1:F:2:VAL:HG22	1:F:43:GLY:C	2.43	0.43
1:G:314:GLN:OE1	1:G:380:THR:CG2	2.67	0.43
1:B:95:LEU:C	1:B:95:LEU:CD2	2.87	0.43
1:A:14:THR:CG2	1:A:366:ASP:HB2	2.49	0.43
1:A:259:GLY:HA3	1:B:66:MET:HE3	2.01	0.43
1:A:272:LYS:CG	1:A:320:MET:HE1	2.47	0.43
1:C:82:LEU:HG	1:C:95:LEU:CD1	2.49	0.43
1:C:259:GLY:HA3	1:D:66:MET:HE3	1.97	0.43
1:D:103:ASN:O	1:D:104:ALA:C	2.61	0.43
1:E:160:CYS:HB2	1:E:161:PRO:HD2	2.01	0.43
1:E:235:ASN:OD1	1:E:238:GLU:HB2	2.19	0.43
1:A:337:VAL:HG13	1:B:236:TRP:HB3	2.00	0.43
1:C:240:ALA:O	1:C:244:VAL:HG13	2.18	0.43
1:D:333:PHE:HB2	1:E:233:TYR:CZ	2.54	0.43
1:E:56:LEU:HD22	1:E:77:ILE:HD12	2.01	0.43
1:G:82:LEU:HD23	1:G:87:ARG:CD	2.49	0.43
1:A:57:ALA:CB	1:A:65:MET:HE2	2.49	0.43
1:A:206:ALA:HB1	1:A:274:LEU:O	2.19	0.43
1:A:365:TRP:CE2	1:A:367:ASN:HB2	2.53	0.43
1:B:2:VAL:HG21	1:B:43:GLY:CA	2.47	0.43
1:B:400:GLU:O	1:B:404:ALA:CB	2.61	0.43
1:C:10:HIS:HB3	1:C:367:ASN:OD1	2.19	0.43
1:E:186:ILE:CG2	1:E:190:MET:HE3	2.48	0.43
1:B:348:GLY:HA2	1:B:352:ARG:HA	2.00	0.43
1:F:109:ASP:O	1:F:113:GLN:HB2	2.18	0.43
1:F:153:ILE:HG22	1:F:158:PHE:HD1	1.82	0.43
1:F:240:ALA:O	1:F:244:VAL:HG13	2.19	0.43
1:G:327:ARG:O	1:G:364:ILE:HA	2.19	0.43
1:D:176:ILE:HG12	1:D:388:LEU:HD22	2.01	0.42
1:F:82:LEU:HD21	1:F:95:LEU:CD1	2.49	0.42
1:F:180:LEU:HD21	1:F:389:ALA:HA	2.01	0.42
1:G:315:PHE:CD2	1:G:379:MET:CE	3.01	0.42
1:B:321:TYR:CD1	1:B:353:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:260:SER:HB2	1:G:363:PRO:HA	2.01	0.42
1:D:315:PHE:CD2	1:D:379:MET:HE1	2.54	0.42
1:E:183:LEU:CD2	1:E:381:MET:HE1	2.35	0.42
1:F:315:PHE:HA	1:F:379:MET:CE	2.45	0.42
1:G:93:THR:HG21	1:G:147:SER:HB2	2.00	0.42
1:G:177:ASN:O	1:G:178:ASN:C	2.63	0.42
1:B:82:LEU:HB2	1:B:85:ALA:HB3	2.02	0.42
1:A:3:LEU:HD22	1:A:8:LEU:HB3	2.02	0.42
1:D:321:TYR:CE2	1:D:353:LEU:HD22	2.54	0.42
1:C:114:GLU:OE1	1:C:114:GLU:HA	2.19	0.42
1:D:307:GLY:O	1:D:310:SER:OG	2.37	0.42
1:C:315:PHE:HA	1:C:379:MET:CE	2.44	0.42
1:G:240:ALA:O	1:G:244:VAL:HG13	2.20	0.42
1:G:304:LEU:HD12	1:G:304:LEU:HA	1.94	0.42
1:G:315:PHE:HA	1:G:379:MET:CE	2.49	0.42
1:C:56:LEU:HD22	1:C:77:ILE:HD12	2.01	0.42
1:D:272:LYS:CG	1:D:320:MET:HE1	2.46	0.42
1:F:58:VAL:HG11	1:F:145:TRP:CH2	2.54	0.42
1:G:82:LEU:HD23	1:G:87:ARG:HD3	2.02	0.42
1:A:14:THR:HG21	1:A:366:ASP:HB2	2.01	0.42
1:B:264:THR:O	1:B:264:THR:HG22	2.18	0.42
1:D:65:MET:HE1	1:D:77:ILE:O	2.20	0.42
1:D:304:LEU:HD12	1:D:304:LEU:HA	1.92	0.42
1:A:304:LEU:HD12	1:A:304:LEU:HA	1.91	0.41
1:B:58:VAL:HG13	1:B:79:PHE:HE2	1.85	0.41
1:B:315:PHE:CD2	1:B:379:MET:HE1	2.55	0.41
1:D:89:PRO:HG3	1:D:143:THR:HB	2.02	0.41
1:E:58:VAL:HG11	1:E:145:TRP:CZ2	2.55	0.41
1:E:206:ALA:HB1	1:E:274:LEU:O	2.20	0.41
1:G:352:ARG:NH2	1:G:352:ARG:HB3	2.35	0.41
1:C:354:ASP:HB3	1:D:398:LYS:NZ	2.34	0.41
1:G:343:ILE:O	1:G:345:ASN:N	2.54	0.41
1:D:223:GLN:HE21	1:D:223:GLN:HB2	1.68	0.41
1:E:336:ASP:OD1	1:E:338:ASN:HB2	2.21	0.41
1:G:88:THR:O	1:G:92:VAL:HG23	2.20	0.41
1:D:135:LEU:HD22	1:D:142:GLY:O	2.20	0.41
1:B:180:LEU:HD21	1:B:389:ALA:HA	2.01	0.41
1:B:395:LEU:O	1:B:396:ALA:C	2.63	0.41
1:C:62:GLU:O	1:C:63:SER:C	2.63	0.41
1:D:91:VAL:O	1:D:91:VAL:CG1	2.67	0.41
1:D:403:ARG:HE	1:D:403:ARG:C	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:HD22	1:B:142:GLY:O	2.21	0.41
1:B:266:ASP:HB2	1:B:267:PRO:HD2	2.02	0.41
1:E:162:VAL:O	1:E:205:LEU:HD23	2.19	0.41
1:F:186:ILE:CG2	1:F:190:MET:HE3	2.50	0.41
1:A:265:TYR:CE1	1:A:269:ASP:HB3	2.55	0.41
1:B:15:ASN:OD1	1:B:16:HIS:N	2.54	0.41
1:D:132:LEU:HD23	1:D:132:LEU:HA	1.88	0.41
1:E:315:PHE:CD2	1:E:379:MET:HE1	2.56	0.41
1:F:206:ALA:O	1:F:278:GLY:HA2	2.21	0.41
1:F:272:LYS:CG	1:F:320:MET:HE1	2.50	0.41
1:G:151:GLN:O	1:G:154:ARG:HB3	2.21	0.41
1:G:380:THR:HG23	1:G:381:MET:N	2.35	0.41
1:B:142:GLY:N	2:B:900:GSP:O2B	2.52	0.41
1:B:272:LYS:CG	1:B:320:MET:HE1	2.51	0.41
1:C:259:GLY:O	1:D:67:HIS:NE2	2.54	0.41
1:C:354:ASP:CB	1:D:398:LYS:HZ1	2.34	0.41
1:C:61:ALA:HB2	1:C:87:ARG:HH11	1.86	0.40
1:C:95:LEU:CD2	1:C:107:TYR:CE1	3.04	0.40
1:C:183:LEU:HD22	1:C:381:MET:CE	2.41	0.40
1:F:164:MET:HB2	1:F:208:VAL:HG22	2.03	0.40
1:B:63:SER:HA	1:B:66:MET:HE2	2.03	0.40
1:B:90:SER:O	1:B:94:ASP:HB2	2.21	0.40
1:C:82:LEU:HD11	1:C:91:VAL:CG1	2.42	0.40
1:D:10:HIS:HB3	1:D:367:ASN:OD1	2.21	0.40
1:E:191:ARG:NH1	1:F:411:ASP:HA	2.36	0.40
1:A:341:ASN:O	1:A:345:ASN:CG	2.63	0.40
1:A:397:GLU:O	1:A:398:LYS:C	2.64	0.40
1:B:2:VAL:CG2	1:B:43:GLY:O	2.70	0.40
1:A:266:ASP:HB2	1:A:267:PRO:HD2	2.04	0.40
1:B:393:LYS:O	1:B:394:GLU:C	2.64	0.40
1:C:186:ILE:CG2	1:C:190:MET:HE3	2.51	0.40
1:C:14:THR:HG21	1:C:366:ASP:HB2	2.04	0.40
1:C:183:LEU:HB3	1:C:381:MET:HE1	2.04	0.40
1:C:304:LEU:HD12	1:C:304:LEU:HA	1.91	0.40
1:D:178:ASN:O	1:D:181:VAL:HG22	2.21	0.40
1:G:259:GLY:O	1:G:363:PRO:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	393/421 (93%)	367 (93%)	24 (6%)	2 (0%)	24	60
1	B	396/421 (94%)	366 (92%)	27 (7%)	3 (1%)	16	50
1	C	406/421 (96%)	379 (93%)	22 (5%)	5 (1%)	10	40
1	D	398/421 (94%)	362 (91%)	31 (8%)	5 (1%)	9	38
1	E	391/421 (93%)	361 (92%)	26 (7%)	4 (1%)	12	45
1	F	410/421 (97%)	382 (93%)	23 (6%)	5 (1%)	10	40
1	G	410/421 (97%)	382 (93%)	25 (6%)	3 (1%)	18	53
All	All	2804/2947 (95%)	2599 (93%)	178 (6%)	27 (1%)	12	45

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	63	SER
1	E	99	GLU
1	E	340	GLU
1	F	338	ASN
1	A	62	GLU
1	D	121	ASN
1	D	406	ALA
1	F	331	ALA
1	G	102	PRO
1	G	354	ASP
1	B	121	ASN
1	D	94	ASP
1	B	17	SER
1	C	115	LEU
1	C	331	ALA
1	D	127	ILE
1	F	333	PHE
1	C	340	GLU

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Mol	Chain	Res	Type
1	A	171	GLY
1	B	171	GLY
1	C	171	GLY
1	D	171	GLY
1	E	127	ILE
1	E	171	GLY
1	F	127	ILE
1	F	171	GLY
1	G	171	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/363 (95%)	306 (89%)	38 (11%)	6	25
1	B	344/363 (95%)	301 (88%)	43 (12%)	4	20
1	C	354/363 (98%)	310 (88%)	44 (12%)	4	20
1	D	346/363 (95%)	305 (88%)	41 (12%)	5	22
1	E	340/363 (94%)	302 (89%)	38 (11%)	6	24
1	F	357/363 (98%)	311 (87%)	46 (13%)	4	19
1	G	358/363 (99%)	311 (87%)	47 (13%)	4	19
All	All	2443/2541 (96%)	2146 (88%)	297 (12%)	5	21

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	17	SER
1	A	32	GLN
1	A	65	MET
1	A	68	LEU
1	A	90	SER
1	A	111	LEU
1	A	115	LEU

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Mol	Chain	Res	Type
1	A	120	THR
1	A	125	GLU
1	A	128	VAL
1	A	132	LEU
1	A	150	LEU
1	A	152	LEU
1	A	153	ILE
1	A	165	LEU
1	A	167	SER
1	A	180	LEU
1	A	182	LEU
1	A	184	SER
1	A	205	LEU
1	A	244	VAL
1	A	256	GLU
1	A	273	LEU
1	A	287	ARG
1	A	290	LYS
1	A	304	LEU
1	A	310	SER
1	A	316	GLU
1	A	330	ASN
1	A	337	VAL
1	A	380	THR
1	A	384	ARG
1	A	395	LEU
1	A	400	GLU
1	A	403	ARG
1	A	405	GLU
1	A	407	GLN
1	B	2	VAL
1	B	8	LEU
1	B	16	HIS
1	B	63	SER
1	B	68	LEU
1	B	82	LEU
1	B	93	THR
1	B	94	ASP
1	B	95	LEU
1	B	103	ASN
1	B	111	LEU
1	B	113	GLN

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Mol	Chain	Res	Type
1	B	115	LEU
1	B	128	VAL
1	B	132	LEU
1	B	150	LEU
1	B	152	LEU
1	B	153	ILE
1	B	165	LEU
1	B	167	SER
1	B	180	LEU
1	B	182	LEU
1	B	184	SER
1	B	205	LEU
1	B	223	GLN
1	B	234	VAL
1	B	244	VAL
1	B	264	THR
1	B	273	LEU
1	B	287	ARG
1	B	290	LYS
1	B	295	SER
1	B	304	LEU
1	B	316	GLU
1	B	325	VAL
1	B	336	ASP
1	B	337	VAL
1	B	341	ASN
1	B	351	LYS
1	B	352	ARG
1	B	380	THR
1	B	384	ARG
1	B	408	ARG
1	C	8	LEU
1	C	62	GLU
1	C	63	SER
1	C	68	LEU
1	C	87	ARG
1	C	93	THR
1	C	105	ASN
1	C	111	LEU
1	C	115	LEU
1	C	121	ASN
1	C	128	VAL

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Mol	Chain	Res	Type
1	C	132	LEU
1	C	150	LEU
1	C	152	LEU
1	C	153	ILE
1	C	165	LEU
1	C	167	SER
1	C	180	LEU
1	C	182	LEU
1	C	184	SER
1	C	205	LEU
1	C	234	VAL
1	C	235	ASN
1	C	244	VAL
1	C	268	SER
1	C	273	LEU
1	C	287	ARG
1	C	292	ASP
1	C	304	LEU
1	C	310	SER
1	C	316	GLU
1	C	325	VAL
1	C	330	ASN
1	C	337	VAL
1	C	351	LYS
1	C	356	ILE
1	C	368	GLU
1	C	380	THR
1	C	384	ARG
1	C	400	GLU
1	C	405	GLU
1	C	409	LYS
1	C	415	VAL
1	C	416	ASP
1	D	8	LEU
1	D	68	LEU
1	D	82	LEU
1	D	87	ARG
1	D	97	ASP
1	D	100	THR
1	D	108	LEU
1	D	109	ASP
1	D	111	LEU

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Mol	Chain	Res	Type
1	D	115	LEU
1	D	118	LYS
1	D	126	VAL
1	D	128	VAL
1	D	132	LEU
1	D	150	LEU
1	D	152	LEU
1	D	153	ILE
1	D	165	LEU
1	D	167	SER
1	D	180	LEU
1	D	182	LEU
1	D	184	SER
1	D	205	LEU
1	D	228	ASP
1	D	232	ARG
1	D	244	VAL
1	D	256	GLU
1	D	263	VAL
1	D	273	LEU
1	D	287	ARG
1	D	299	SER
1	D	304	LEU
1	D	310	SER
1	D	316	GLU
1	D	368	GLU
1	D	380	THR
1	D	384	ARG
1	D	393	LYS
1	D	401	GLN
1	D	403	ARG
1	D	407	GLN
1	E	8	LEU
1	E	62	GLU
1	E	63	SER
1	E	68	LEU
1	E	82	LEU
1	E	87	ARG
1	E	88	THR
1	E	103	ASN
1	E	111	LEU
1	E	122	GLU

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Mol	Chain	Res	Type
1	E	128	VAL
1	E	132	LEU
1	E	150	LEU
1	E	152	LEU
1	E	153	ILE
1	E	165	LEU
1	E	167	SER
1	E	180	LEU
1	E	182	LEU
1	E	184	SER
1	E	205	LEU
1	E	223	GLN
1	E	244	VAL
1	E	257	ASN
1	E	273	LEU
1	E	287	ARG
1	E	296	LEU
1	E	304	LEU
1	E	310	SER
1	E	316	GLU
1	E	351	LYS
1	E	368	GLU
1	E	380	THR
1	E	384	ARG
1	E	390	ARG
1	E	395	LEU
1	E	397	GLU
1	E	400	GLU
1	F	2	VAL
1	F	8	LEU
1	F	68	LEU
1	F	78	HIS
1	F	80	ASP
1	F	82	LEU
1	F	88	THR
1	F	95	LEU
1	F	103	ASN
1	F	111	LEU
1	F	115	LEU
1	F	128	VAL
1	F	132	LEU
1	F	150	LEU

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Mol	Chain	Res	Type
1	F	152	LEU
1	F	153	ILE
1	F	165	LEU
1	F	167	SER
1	F	180	LEU
1	F	182	LEU
1	F	205	LEU
1	F	244	VAL
1	F	256	GLU
1	F	266	ASP
1	F	268	SER
1	F	273	LEU
1	F	287	ARG
1	F	299	SER
1	F	304	LEU
1	F	316	GLU
1	F	330	ASN
1	F	335	LYS
1	F	337	VAL
1	F	351	LYS
1	F	354	ASP
1	F	356	ILE
1	F	380	THR
1	F	384	ARG
1	F	397	GLU
1	F	399	GLN
1	F	401	GLN
1	F	403	ARG
1	F	407	GLN
1	F	408	ARG
1	F	415	VAL
1	F	421	THR
1	G	2	VAL
1	G	8	LEU
1	G	65	MET
1	G	68	LEU
1	G	80	ASP
1	G	82	LEU
1	G	87	ARG
1	G	91	VAL
1	G	95	LEU
1	G	99	GLU

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Mol	Chain	Res	Type
1	G	111	LEU
1	G	128	VAL
1	G	132	LEU
1	G	150	LEU
1	G	152	LEU
1	G	153	ILE
1	G	165	LEU
1	G	167	SER
1	G	180	LEU
1	G	182	LEU
1	G	184	SER
1	G	205	LEU
1	G	226	THR
1	G	234	VAL
1	G	244	VAL
1	G	266	ASP
1	G	273	LEU
1	G	287	ARG
1	G	294	HIS
1	G	295	SER
1	G	298	ASN
1	G	299	SER
1	G	304	LEU
1	G	316	GLU
1	G	337	VAL
1	G	351	LYS
1	G	355	GLU
1	G	366	ASP
1	G	368	GLU
1	G	380	THR
1	G	384	ARG
1	G	390	ARG
1	G	399	GLN
1	G	407	GLN
1	G	410	GLN
1	G	416	ASP
1	G	417	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN

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Mol	Chain	Res	Type
1	A	70	ASN
1	A	151	GLN
1	A	215	GLN
1	A	294	HIS
1	B	19	ASN
1	B	35	ASN
1	B	59	ASN
1	B	215	GLN
1	B	399	GLN
1	C	19	ASN
1	C	70	ASN
1	C	215	GLN
1	C	257	ASN
1	D	19	ASN
1	D	70	ASN
1	D	103	ASN
1	D	215	GLN
1	D	223	GLN
1	E	16	HIS
1	E	19	ASN
1	E	215	GLN
1	F	19	ASN
1	F	70	ASN
1	F	103	ASN
1	F	215	GLN
1	F	410	GLN
1	G	16	HIS
1	G	19	ASN
1	G	70	ASN
1	G	78	HIS
1	G	215	GLN
1	G	410	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GSP	C	900	3	33,34,34	1.90	6 (18%)	47,54,54	1.68	10 (21%)
2	GSP	B	900	3	33,34,34	2.10	5 (15%)	47,54,54	1.88	10 (21%)
2	GSP	G	900	3	33,34,34	1.92	2 (6%)	47,54,54	1.77	12 (25%)
2	GSP	D	900	3	33,34,34	1.98	3 (9%)	47,54,54	1.80	11 (23%)
2	GSP	F	900	3	33,34,34	1.97	1 (3%)	47,54,54	2.08	19 (40%)
2	GSP	A	900	3	33,34,34	2.20	4 (12%)	47,54,54	1.78	12 (25%)
2	GSP	E	900	3	33,34,34	1.98	4 (12%)	47,54,54	1.73	10 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSP	C	900	3	-	0/21/38/38	0/3/3/3
2	GSP	B	900	3	-	5/21/38/38	0/3/3/3
2	GSP	G	900	3	-	4/21/38/38	0/3/3/3
2	GSP	D	900	3	-	6/21/38/38	0/3/3/3
2	GSP	F	900	3	-	3/21/38/38	0/3/3/3
2	GSP	A	900	3	-	4/21/38/38	0/3/3/3
2	GSP	E	900	3	-	5/21/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	GSP	PG-S1G	-10.84	1.67	1.90
2	B	900	GSP	PG-S1G	-10.16	1.68	1.90
2	F	900	GSP	PG-S1G	-9.93	1.69	1.90
2	G	900	GSP	PG-S1G	-9.74	1.69	1.90
2	E	900	GSP	PG-S1G	-9.68	1.69	1.90
2	D	900	GSP	PG-S1G	-9.53	1.70	1.90
2	C	900	GSP	PG-S1G	-8.53	1.72	1.90
2	C	900	GSP	PB-O3A	2.86	1.62	1.59
2	D	900	GSP	PB-O3A	2.82	1.62	1.59
2	C	900	GSP	C2-N3	2.67	1.39	1.33
2	B	900	GSP	C5-N7	-2.65	1.33	1.39
2	A	900	GSP	PB-O3A	2.63	1.62	1.59
2	E	900	GSP	C5-N7	-2.63	1.33	1.39
2	A	900	GSP	PB-O3B	2.53	1.62	1.59
2	C	900	GSP	PA-O3A	2.43	1.62	1.59
2	E	900	GSP	C2-N3	2.38	1.38	1.33
2	A	900	GSP	PA-O3A	2.28	1.62	1.59
2	C	900	GSP	C5-N7	-2.23	1.34	1.39
2	D	900	GSP	PB-O3B	2.18	1.61	1.59
2	B	900	GSP	PB-O3B	2.16	1.61	1.59
2	E	900	GSP	C5-C6	-2.16	1.36	1.44
2	B	900	GSP	PB-O3A	2.13	1.61	1.59
2	C	900	GSP	C5-C6	-2.07	1.36	1.44
2	B	900	GSP	C5-C6	-2.05	1.37	1.44
2	G	900	GSP	PB-O3B	2.00	1.61	1.59

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	GSP	C5-C4-N3	-5.46	119.69	128.39
2	F	900	GSP	C2'-C1'-N9	5.39	128.26	113.25
2	G	900	GSP	C2-N3-C4	5.12	121.11	112.30
2	B	900	GSP	C2-N3-C4	5.09	121.07	112.30
2	F	900	GSP	C2-N3-C4	5.02	120.94	112.30
2	G	900	GSP	C5-C4-N3	-5.02	120.41	128.39
2	D	900	GSP	C5-C4-N3	-4.98	120.46	128.39
2	C	900	GSP	C5-C4-N3	-4.96	120.50	128.39
2	A	900	GSP	C2-N3-C4	4.81	120.58	112.30
2	A	900	GSP	C5-C4-N3	-4.52	121.20	128.39
2	D	900	GSP	C2-N3-C4	4.40	119.87	112.30
2	E	900	GSP	C5-C4-N3	-4.32	121.52	128.39
2	F	900	GSP	C5-C4-N3	-4.30	121.55	128.39
2	E	900	GSP	PB-O3B-PG	-4.27	117.56	133.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	GSP	C2-N3-C4	3.92	119.05	112.30
2	D	900	GSP	PB-O3B-PG	-3.88	118.99	133.17
2	E	900	GSP	C2-N3-C4	3.79	118.82	112.30
2	C	900	GSP	N9-C4-N3	3.75	133.44	125.95
2	F	900	GSP	PB-O3B-PG	-3.70	119.63	133.17
2	F	900	GSP	O4'-C1'-N9	-3.54	100.34	108.36
2	B	900	GSP	N9-C4-N3	3.53	133.01	125.95
2	D	900	GSP	C2-N1-C6	-3.47	118.82	125.11
2	F	900	GSP	O2A-PA-O3A	3.26	116.08	107.27
2	C	900	GSP	PB-O3B-PG	-3.24	121.32	133.17
2	F	900	GSP	N2-C2-N1	3.19	123.49	116.76
2	B	900	GSP	O6-C6-C5	-3.17	118.16	126.53
2	B	900	GSP	C2-N1-C6	-3.14	119.42	125.11
2	E	900	GSP	O6-C6-C5	-3.14	118.26	126.53
2	B	900	GSP	N9-C8-N7	-3.13	107.59	113.40
2	A	900	GSP	C5-C6-N1	3.09	121.11	113.25
2	A	900	GSP	C2-N1-C6	-3.08	119.52	125.11
2	B	900	GSP	C5-C6-N1	3.03	120.97	113.25
2	C	900	GSP	O6-C6-C5	-3.01	118.60	126.53
2	D	900	GSP	O2B-PB-O3A	2.99	115.36	107.27
2	C	900	GSP	O2A-PA-O3A	2.97	115.31	107.27
2	E	900	GSP	C2-N1-C6	-2.95	119.75	125.11
2	D	900	GSP	O3A-PA-O1A	-2.95	101.84	110.70
2	A	900	GSP	N2-C2-N1	2.90	122.89	116.76
2	A	900	GSP	O3G-PG-O3B	2.90	114.31	104.64
2	B	900	GSP	C8-N7-C5	2.88	109.38	104.26
2	D	900	GSP	N9-C4-N3	2.85	131.65	125.95
2	B	900	GSP	O3G-PG-O3B	2.85	114.15	104.64
2	G	900	GSP	C2-N1-C6	-2.84	119.97	125.11
2	D	900	GSP	O6-C6-C5	-2.77	119.22	126.53
2	A	900	GSP	N9-C8-N7	-2.77	108.27	113.40
2	G	900	GSP	PB-O3B-PG	-2.76	123.08	133.17
2	E	900	GSP	N9-C4-N3	2.73	131.42	125.95
2	C	900	GSP	C5-C6-N1	2.73	120.20	113.25
2	C	900	GSP	C2-N1-C6	-2.69	120.23	125.11
2	E	900	GSP	O2A-PA-O3A	2.68	114.51	107.27
2	A	900	GSP	C6-C5-N7	2.67	135.15	130.29
2	G	900	GSP	N9-C8-N7	-2.63	108.52	113.40
2	E	900	GSP	C5-C6-N1	2.62	119.92	113.25
2	G	900	GSP	C8-N7-C5	2.61	108.90	104.26
2	D	900	GSP	N9-C8-N7	-2.60	108.58	113.40
2	G	900	GSP	C2'-C1'-N9	2.51	120.22	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	900	GSP	N2-C2-N1	2.47	121.97	116.76
2	C	900	GSP	N9-C8-N7	-2.41	108.93	113.40
2	D	900	GSP	C5-C6-N1	2.39	119.33	113.25
2	G	900	GSP	N9-C4-N3	2.38	130.72	125.95
2	F	900	GSP	N1-C2-N3	-2.38	118.97	123.32
2	E	900	GSP	N9-C8-N7	-2.37	109.00	113.40
2	G	900	GSP	C4-C5-N7	-2.37	106.91	110.67
2	A	900	GSP	C8-N7-C5	2.31	108.38	104.26
2	F	900	GSP	C1'-N9-C8	2.30	133.26	126.73
2	F	900	GSP	C2'-C3'-C4'	2.27	107.00	102.61
2	G	900	GSP	C5-C6-N1	2.26	119.00	113.25
2	F	900	GSP	C2-N1-C6	-2.25	121.02	125.11
2	F	900	GSP	O2A-PA-O5'	2.23	117.68	107.57
2	F	900	GSP	O6-C6-C5	-2.21	120.71	126.53
2	A	900	GSP	O6-C6-C5	-2.20	120.72	126.53
2	B	900	GSP	N1-C2-N3	-2.19	119.31	123.32
2	F	900	GSP	C5-C6-N1	2.19	118.83	113.25
2	C	900	GSP	C8-N7-C5	2.17	108.13	104.26
2	F	900	GSP	N9-C8-N7	-2.16	109.40	113.40
2	F	900	GSP	C8-N7-C5	2.14	108.08	104.26
2	F	900	GSP	C1'-N9-C4	-2.13	120.20	126.49
2	D	900	GSP	C8-N7-C5	2.13	108.05	104.26
2	A	900	GSP	C4-C5-N7	-2.13	107.30	110.67
2	F	900	GSP	C4-C5-N7	-2.11	107.32	110.67
2	A	900	GSP	N9-C4-N3	2.11	130.17	125.95
2	F	900	GSP	C6-C5-N7	2.03	133.99	130.29
2	E	900	GSP	O2G-PG-O3B	2.01	111.34	104.64
2	G	900	GSP	O6-C6-C5	-2.00	121.25	126.53

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	GSP	PB-O3B-PG-O2G
2	A	900	GSP	PB-O3B-PG-O3G
2	A	900	GSP	C5'-O5'-PA-O2A
2	A	900	GSP	C5'-O5'-PA-O3A
2	B	900	GSP	PB-O3B-PG-O3G
2	B	900	GSP	O4'-C4'-C5'-O5'
2	D	900	GSP	C5'-O5'-PA-O1A
2	D	900	GSP	C5'-O5'-PA-O2A
2	D	900	GSP	C5'-O5'-PA-O3A

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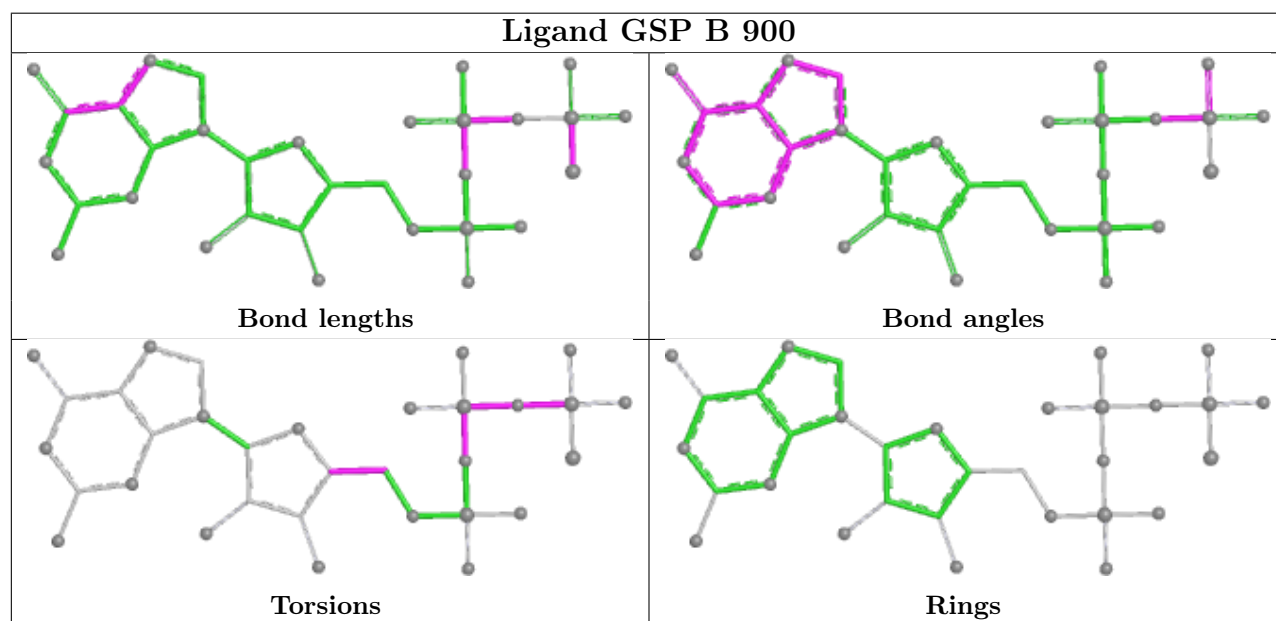
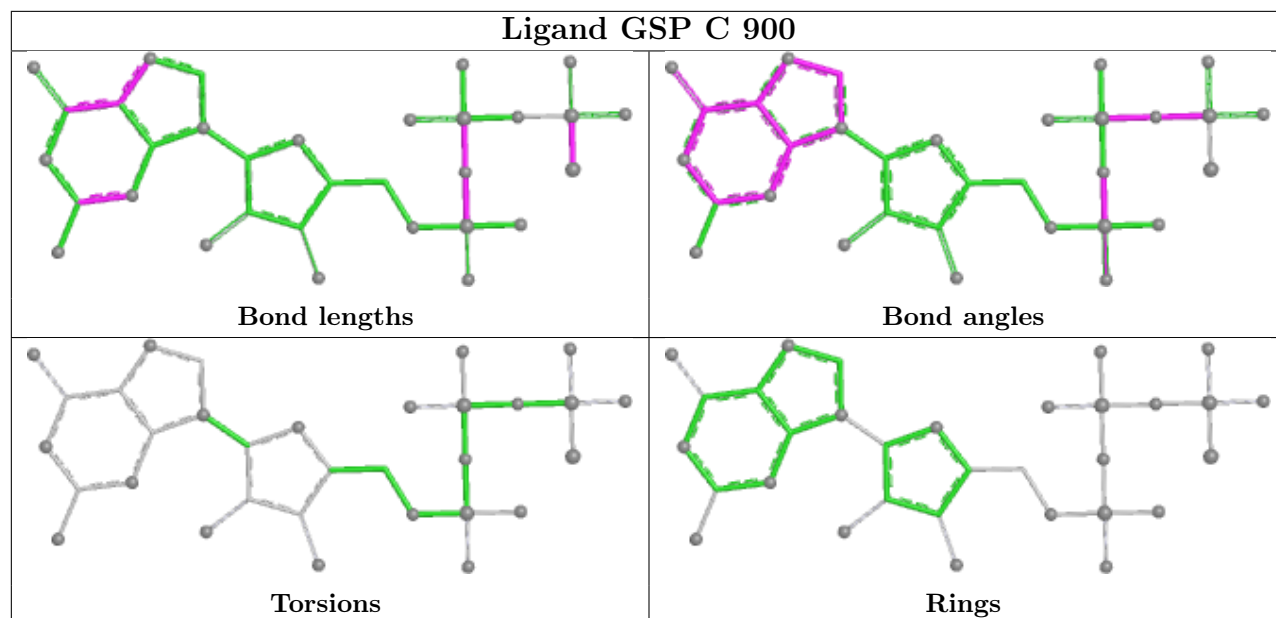
Mol	Chain	Res	Type	Atoms
2	E	900	GSP	C5'-O5'-PA-O1A
2	E	900	GSP	C5'-O5'-PA-O2A
2	G	900	GSP	C5'-O5'-PA-O2A
2	G	900	GSP	C5'-O5'-PA-O3A
2	B	900	GSP	C3'-C4'-C5'-O5'
2	E	900	GSP	O4'-C4'-C5'-O5'
2	B	900	GSP	PG-O3B-PB-O1B
2	D	900	GSP	PB-O3A-PA-O1A
2	F	900	GSP	PB-O3A-PA-O2A
2	G	900	GSP	O4'-C4'-C5'-O5'
2	E	900	GSP	C5'-O5'-PA-O3A
2	F	900	GSP	C5'-O5'-PA-O3A
2	G	900	GSP	C5'-O5'-PA-O1A
2	D	900	GSP	PA-O3A-PB-O2B
2	D	900	GSP	PB-O3B-PG-O3G
2	B	900	GSP	PA-O3A-PB-O2B
2	F	900	GSP	PB-O3A-PA-O1A
2	E	900	GSP	C3'-C4'-C5'-O5'

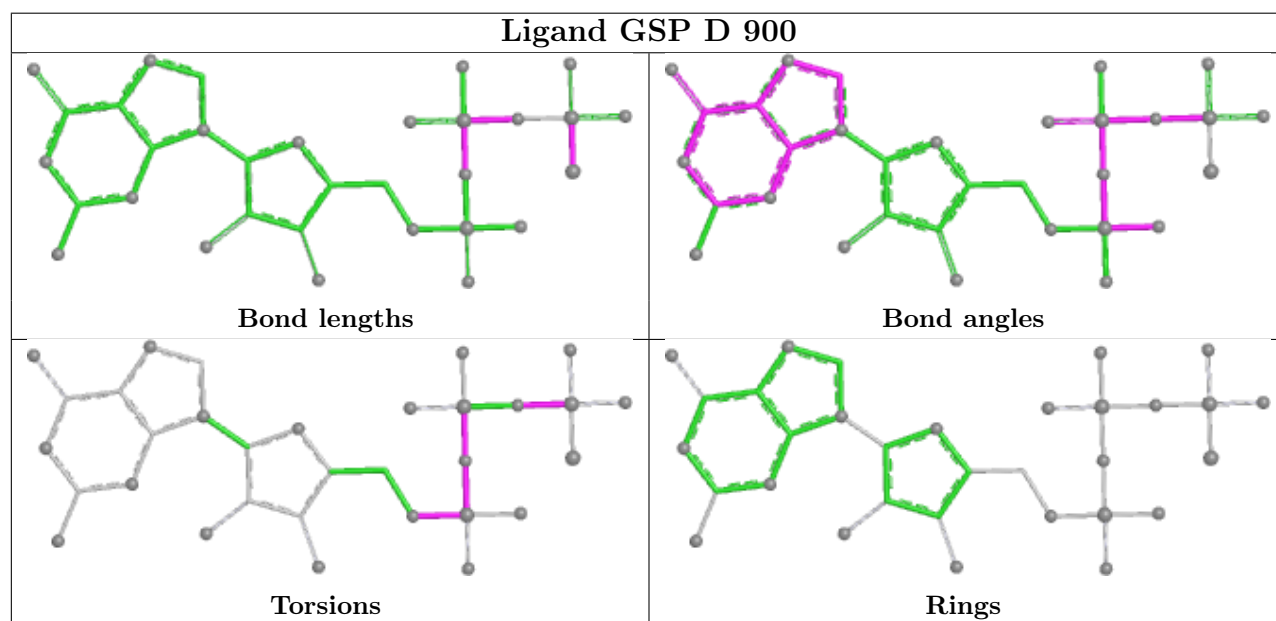
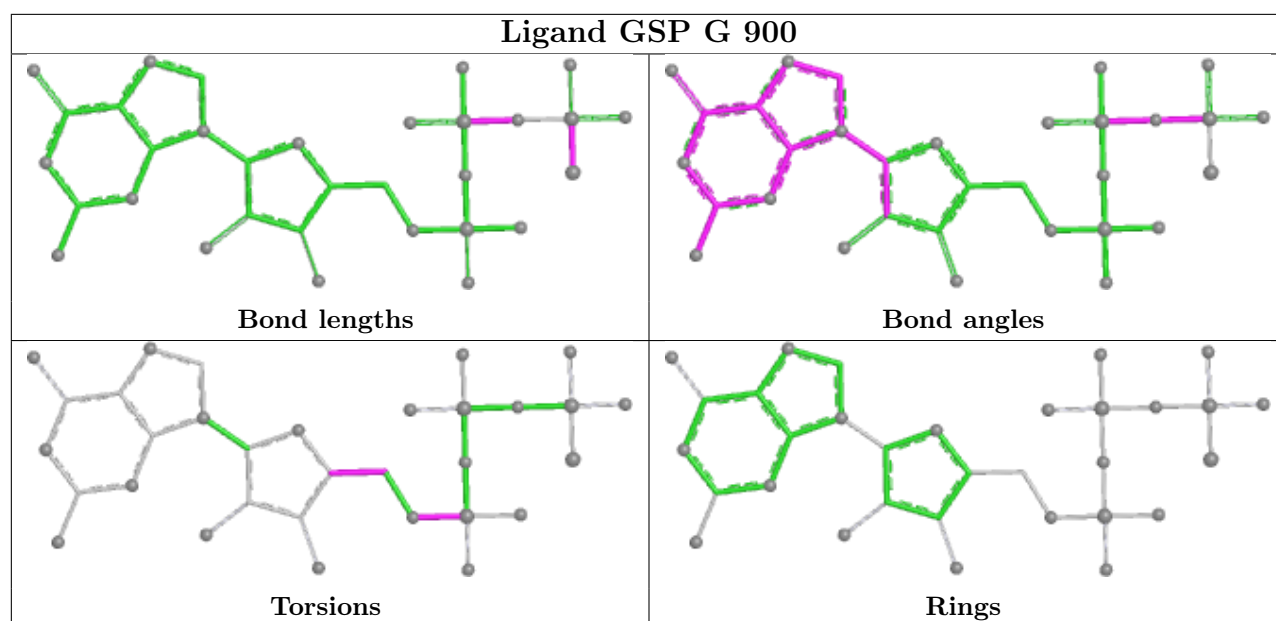
There are no ring outliers.

3 monomers are involved in 4 short contacts:

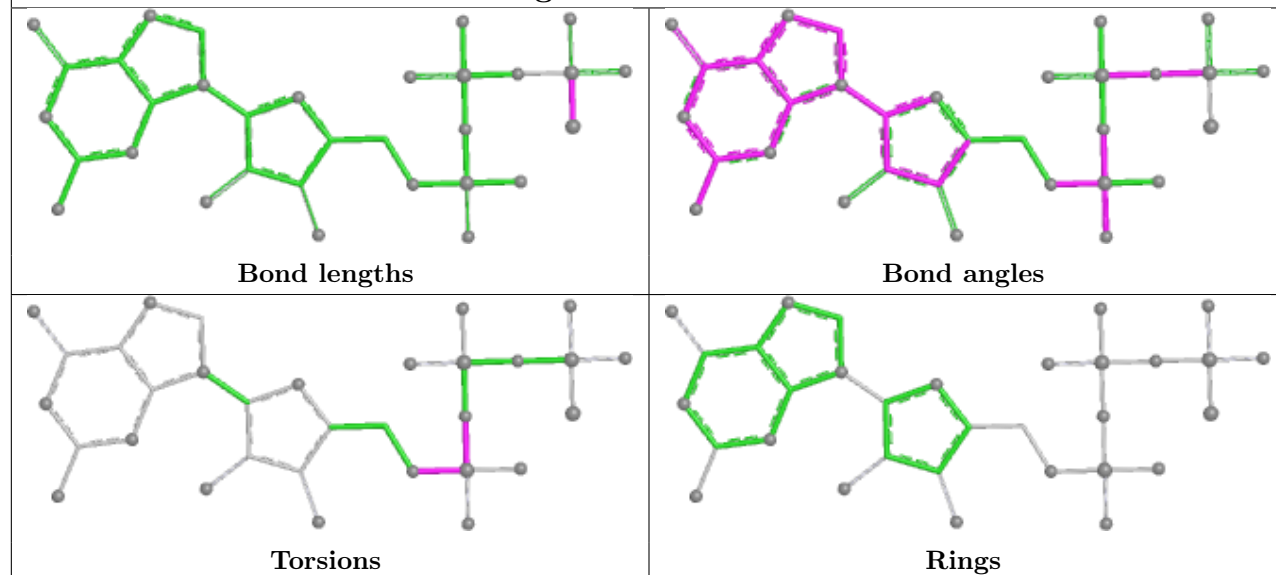
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	GSP	2	0
2	A	900	GSP	1	0
2	E	900	GSP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

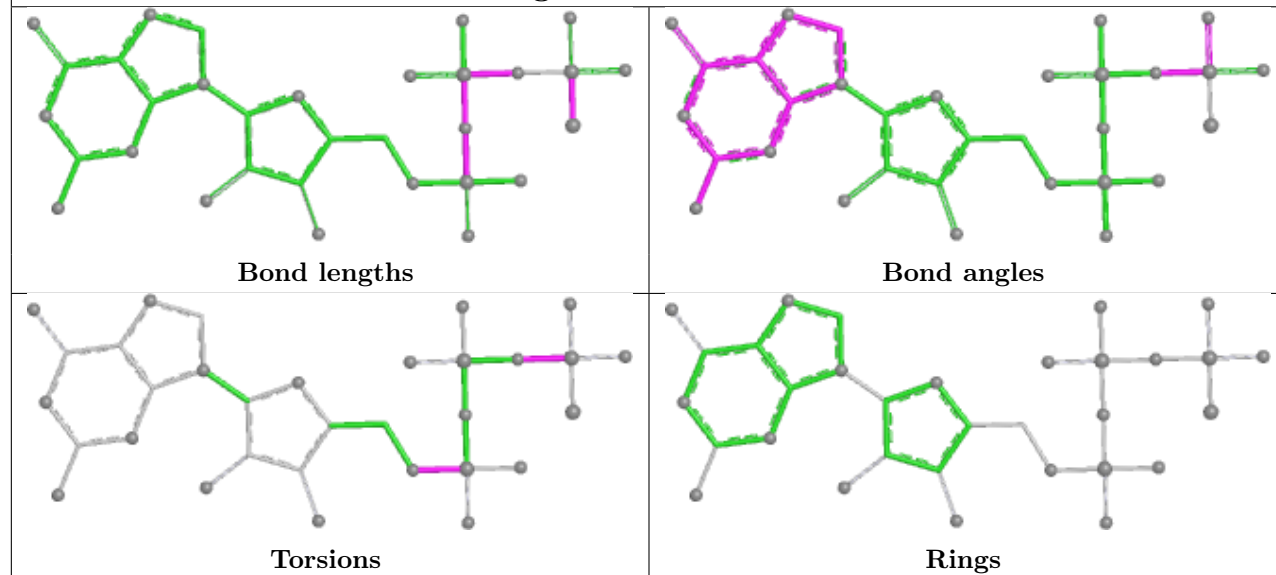


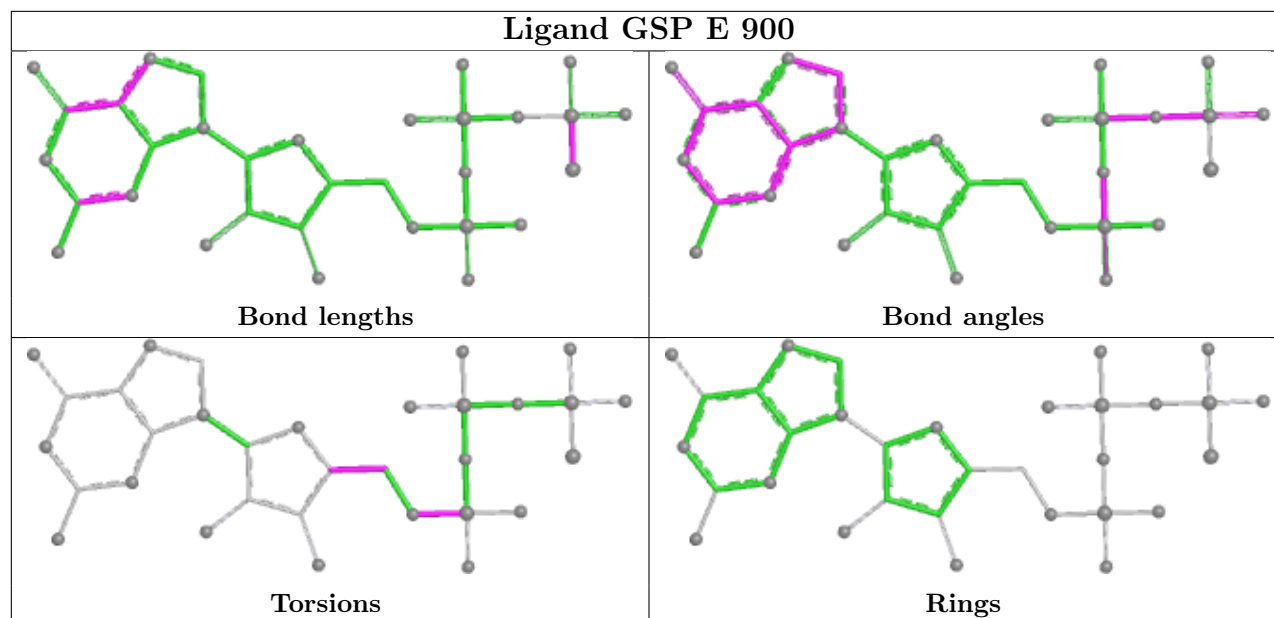


Ligand GSP F 900



Ligand GSP A 900





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	399/421 (94%)	-0.02	4 (1%) 79 59	8, 29, 55, 66	0
1	B	400/421 (95%)	0.07	0 100 100	8, 29, 52, 78	0
1	C	410/421 (97%)	0.07	4 (0%) 79 59	8, 28, 46, 55	0
1	D	402/421 (95%)	0.01	2 (0%) 87 72	8, 27, 44, 64	0
1	E	395/421 (93%)	0.04	6 (1%) 72 49	8, 24, 41, 57	0
1	F	414/421 (98%)	0.05	3 (0%) 84 66	8, 26, 40, 48	0
1	G	414/421 (98%)	0.01	1 (0%) 91 83	8, 28, 42, 48	0
All	All	2834/2947 (96%)	0.03	20 (0%) 84 66	8, 27, 45, 78	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	172	ASP	3.5
1	E	306	GLU	2.6
1	F	171	GLY	2.6
1	E	2	VAL	2.5
1	D	174	ASP	2.5
1	A	85	ALA	2.5
1	G	221	GLU	2.4
1	E	173	PRO	2.4
1	A	82	LEU	2.4
1	F	172	ASP	2.3
1	C	6	ASN	2.3
1	E	99	GLU	2.2
1	C	192	GLU	2.1
1	E	404	ALA	2.1
1	D	99	GLU	2.1
1	A	222	SER	2.1
1	C	11	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	201	ASP	2.0
1	F	173	PRO	2.0
1	A	221	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

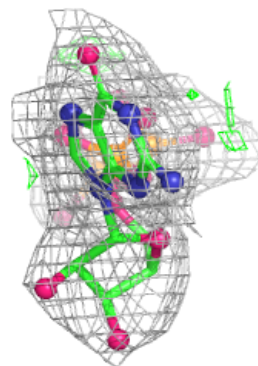
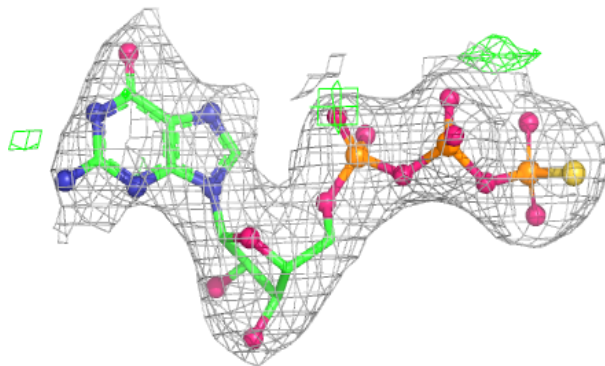
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	999	1/1	0.93	0.14	17,17,17,17	0
3	MG	E	999	1/1	0.95	0.14	2,2,2,2	0
2	GSP	A	900	32/32	0.96	0.08	13,19,23,23	0
3	MG	C	999	1/1	0.96	0.14	2,2,2,2	0
2	GSP	C	900	32/32	0.96	0.07	11,13,16,18	0
3	MG	G	999	1/1	0.96	0.11	17,17,17,17	0
2	GSP	F	900	32/32	0.97	0.06	2,4,6,7	0
3	MG	D	999	1/1	0.97	0.15	5,5,5,5	0
2	GSP	D	900	32/32	0.97	0.07	5,9,10,12	0
3	MG	F	999	1/1	0.97	0.14	2,2,2,2	0
3	MG	B	999	1/1	0.97	0.14	12,12,12,12	0
2	GSP	B	900	32/32	0.98	0.06	2,5,7,11	0
2	GSP	G	900	32/32	0.98	0.06	3,9,12,14	0
2	GSP	E	900	32/32	0.98	0.06	2,3,6,8	0

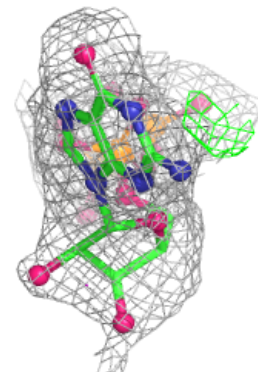
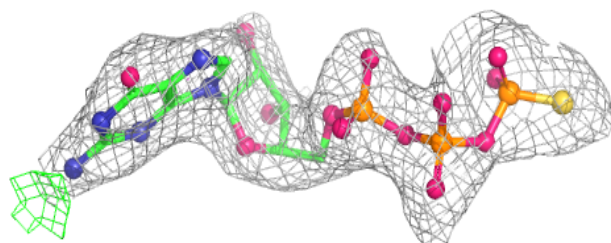
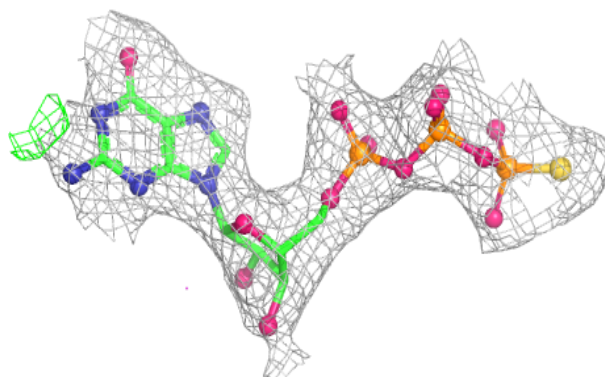
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GSP A 900:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

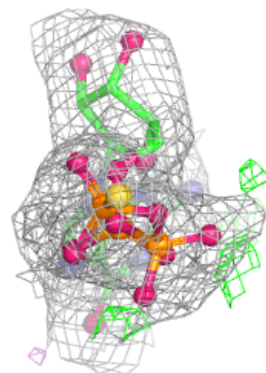
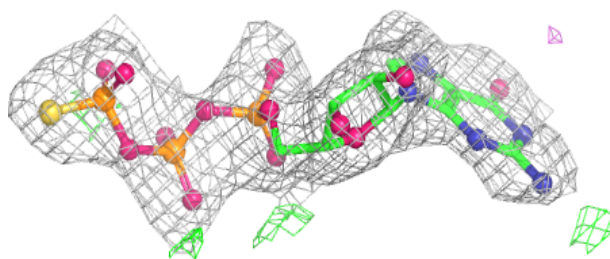
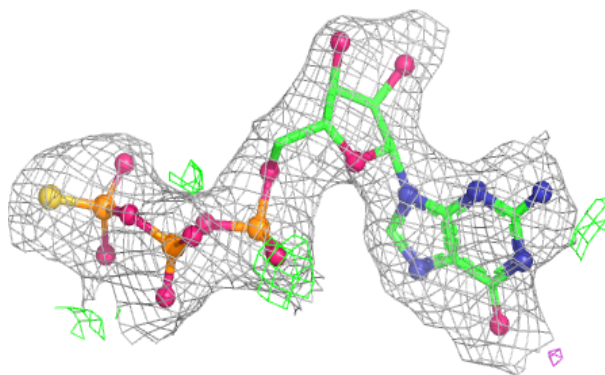
**Electron density around GSP C 900:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

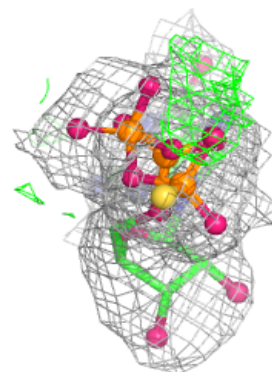
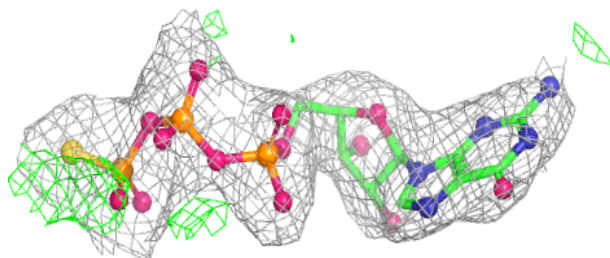
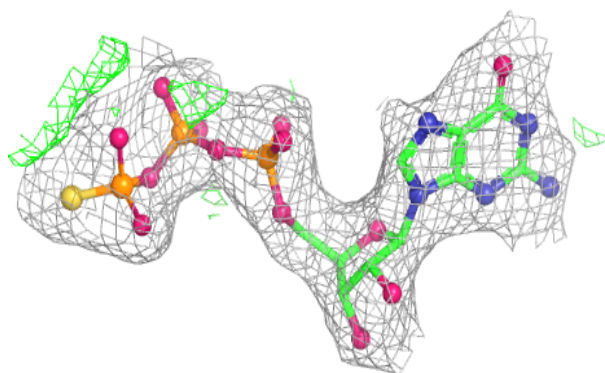


Electron density around GSP F 900:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

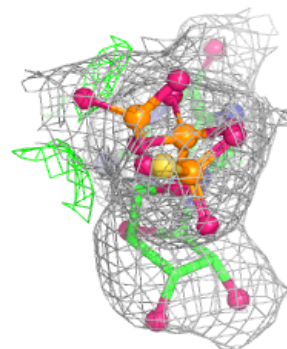
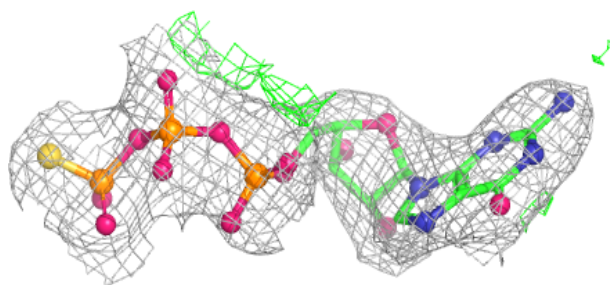
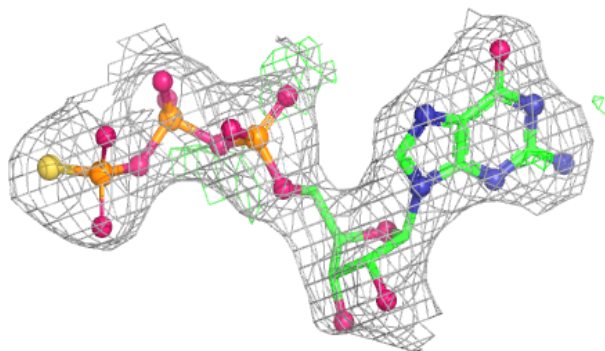
**Electron density around GSP D 900:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

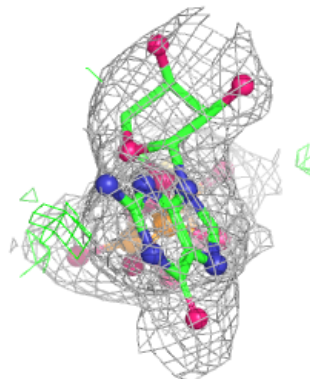
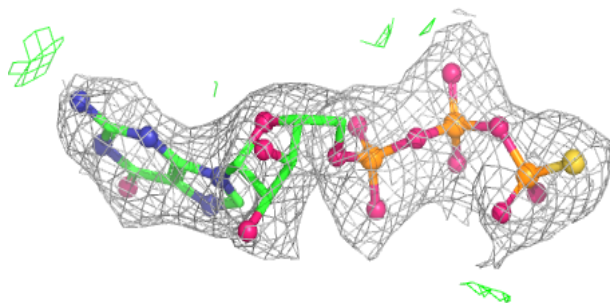
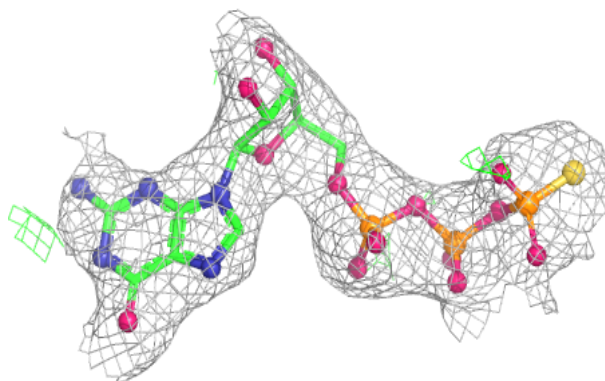


Electron density around GSP B 900:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

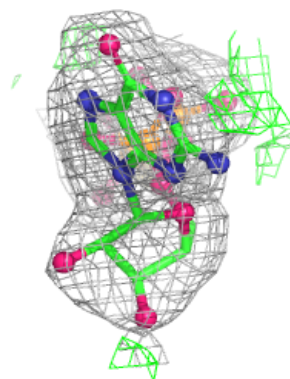
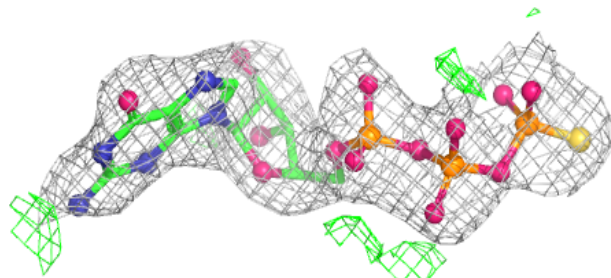
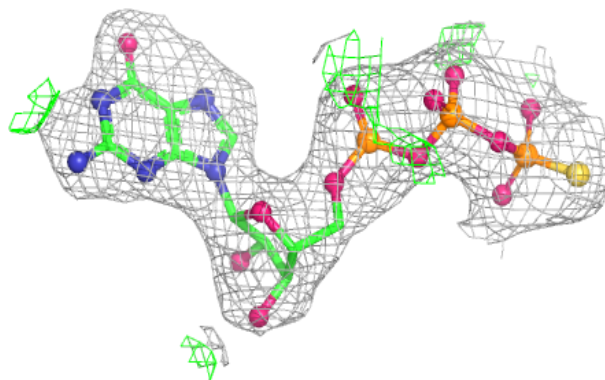
**Electron density around GSP G 900:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GSP E 900:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.